PARTICLES AND QUANTUM FIELDS

Particles and Quantum Fields

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Preface

This book arose from lectures I gave at the Free University Berlin over a number of years. The lectures were intended as two-semester+ introductions to graduate students who intended to start theoretical research work either in many-body physics or in particle physics.

Being a general broadly-based introduction, the book requires extension into two directions which have to be subjects of continuing specialized courses. What is needed is

- a more detailed account of the exciting developments in nonabelian gauge theories which has taken place over the last decade establishimg quantum chromodynamics as a most probably true theory of strong interactions.
- a proper presentation of the field-theoretic explanations of the critical properties of many-body systems near second-order phase transitions.

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Contents

1 Fundamentals **1**

1.1 Quantum Mechanics 1
1.2 Dirac's Bra-Ket Formalism 8
1.3 Observables 16
1.4 Time Evolution Operator 20
1.5 Properties of Time Evolution Operator 28
1.6 Heisenberg Picture of Quantum Mechanics 33
1.7 Classical and Quantum Statistics 35
Notes and References 41

2 Field Formulation of Many-Body Quantum Physics **43**

2.1 Mechanics and Quantum Mechanics for n Distinguishable Nonrelativistic Particles 43
2.2 Identical Particles — Bosons and Fermions 46
2.3 Creation and Annihilation Operators for Bosons 51
2.4 Schrödinger Equation of Noninteracting Bosons in Terms of Creation 56
2.5 Second Quantization and Symmetrized Product Representation . . . 57
2.6 Bosons with Two-Body Interactions 61
2.7 Quantum Field Formulation of Many-Boson Schrödinger Equations . 63
2.8 Canonical Formalism in Quantum Field Theory 65
2.9 More General Creation and Annihilation Operators 70
2.10 Quantum Field Formulation of Many-Fermion Schrödinger Equations 72
2.11 Free Nonrelativistic Particles and Fields 74
2.12 Second-Quantized Current Conservation Law 77
2.13 Free-Particle Propagator 77
2.14 Quantum Statistic of Free Particles 80
  2.14.1 Thermodynamic Quantities 80
  2.14.2 The Degenerate Fermi Gas Near $T = 0$ 86
  2.14.3 Degenerate Bose Gas Near $T = 0$ 91
  2.14.4 High Temperatures 96
2.15 Temperature Green Functions of Free Particles 97
2.16 Calculating the Matsubara Sum via Poissons Formula 101
Appendix 2A Permutation Group and Representations 103
Notes and References 109

3 Relativistic Free Fields 111

3.1 RELATIVISTIC PARTICLES 111
3.2 DIFFERENTIAL OPERATORS FOR LORENTZ TRANSFORMATIONS 118
3.3 SPACE INVERSION AND TIME REVERSAL 127
3.4 RELATIVISTIC FREE SCALAR FIELDS 128
3.5 OTHER SYMMETRIES OF SCALAR ACTION 136
  3.5.1 Translations 136
  3.5.2 Space Inversion 137
  3.5.3 Time Reversal 139
  3.5.4 Charge Conjugation 142
3.6 ELECTROMAGNETIC FIELD 143
  3.6.1 Action and Field Equations 143
  3.6.2 Gauge Invariance 145
  3.6.3 Lorentz Transformation Properties of Electromagnetic Fields 148
3.7 OTHER SYMMETRIES OF ELECTROMAGNETIC ACTION . . . 150
  3.7.1 Translations 150
  3.7.2 Space Inversion, Time Reversal, and Charge Conjugation . . 150
3.8 PLANE-WAVE SOLUTIONS OF MAXWELL'S EQUATIONS . . . 151
3.9 MASSIVE VECTOR FIELDS 155
  3.9.1 Action and Field Equations 155
  3.9.2 Plane Wave Solutions for Massive Vector Fields 156
3.10 GRAVITATIONAL FIELD 160
  3.10.1 Action and Field Equations 160
  3.10.2 Gauge Properties 162
  3.10.3 Lorentz Transformation Properties of Gravitational Field . . 163
  3.10.4 Other Symmetries of Gravitational Action 163
  3.10.5 Translations 163
  3.10.6 Space Inversion, Time Reversal, and Charge Conjugation . . 164
  3.10.7 Gravitational Plane Waves 164
3.11 RELATIVISTIC FREE FERMI FIELDS 167
3.12 SPIN-1/2 FIELDS 168
3.13 OTHER SYMMETRIES OF DIRAC ACTION 178
  3.13.1 Translations 178
  3.13.2 Space Inversion 178
  3.13.3 Charge Conjugation 187
  3.13.4 Time Reversal 190
  3.13.5 Transformation Properties of Currents 192
3.14 MAJORANA FIELDS 193
  3.14.1 Plane-Wave Solutions of Dirac Equation 196
3.15 LORENTZ TRANSFORMATION OF SPINORS 207
3.16 THOMAS PRECESSION 210
  3.16.1 Spin Four-Vector and Little Group 214
3.17 WEYL'S SPINOR CALCULUS 218

3.18 HIGHER-SPIN REPRESENTATIONS 220
  3.18.1 Rotations 220
  3.18.2 Extension to Lorentz Group 223
  3.18.3 Finite Representation Matrices 225
3.19 HIGHER-SPIN FIELDS 231
  3.19.1 Plane-Wave Solutions 233
3.20 VECTOR FIELD AS A HIGHER-SPIN FIELD 235
3.21 RARITA SCHWINGER FIELD FOR SPIN 3/2 236
Appendix 3A Derivation of Baker-Campbell-Hausdorff Formula 237
Appendix 3B Wigner Rotations and Lobatschewksi Geometry of Rapidities 240
Appendix 3C Clebsch-Gordan Coefficients 246
Appendix 3D Spherical Harmonics 251
Notes and References 253

4 Relativistic Fields in External Electromagnetic Field 254
4.1 Minimal Substitution Law and Gauge Invariant Electromagnetic Interaction 254
4.2 Pauli Equation 260
4.3 Relativistic Wave Equations in Coulomb Potential 262
  4.3.1 Reminder of Schrödinger Equation for Coulomb Potential . 262
  4.3.2 Klein-Gordon Field in Coulomb Potential 264
  4.3.3 Dirac Field in Coulomb Potential 265
Appendix 4A Spinor Spherical Harmonics 270

5 Quantization of Relativistic Free Fields 273
5.1 SCALAR FIELDS 274
  5.1.1 Real Case 274
  5.1.2 Field Quantization 274
  5.1.3 Propagator of Free Scalar Particles 279
  5.1.4 Complex Case 282
  5.1.5 Energy of Free Charged Scalar Particles 284
  5.1.6 Behavior under Discrete Symmetries 286
5.2 SPACETIME BEHAVIOR OF PROPAGATORS 292
  5.2.1 Wick Rotation 292
  5.2.2 Feynman Propagator in Minkowski Space 294
  5.2.3 Retarded and Advanced Propagators 297
  5.2.4 Comparison of Singular Functions 301
5.3 FREE DIRAC FIELDS 305
  5.3.1 Field Quantization 305
  5.3.2 Energy of Free Dirac Particles 309
  5.3.3 Lorentz Transformation Properties of Particle States 311
  5.3.4 Behavior under Discrete Symmetries 320
5.4 FREE PHOTON FIELD 324
  5.4.1 Field Quantization 325

- 5.4.2 Covariant Field Quantization 330
- 5.4.3 Behavior under Discrete Symmetries 356
- 5.5 MASSIVE VECTOR BOSONS 357
  - 5.5.1 Field Quantization 358
  - 5.5.2 Energy of Massive Vector Particle 359
  - 5.5.3 Propagator of Massive Vector Particle 361
  - 5.5.4 Behavior under Discrete Symmetry Transformations 365
- 5.6 SPIN-3/2 FIELDS 366
- 5.7 GRAVITONS 368
- 5.8 SPIN-STATISTICS THEOREM 369
- 5.9 CPT THEOREM 372
- 5.10 PHYSICAL CONSEQUENCES OF VACUUM FLUCTUATIONS. CASIMIR EFFECT 373
- 5.11 ZETA FUNCTION REGULARIZATION 378
- 5.12 FREE GREEN FUNCTIONS OF n FIELDS 381
  - 5.12.1 Wick's Theorem 386
- 5.13 Functional Form of Wick's Theorem 389
  - 5.13.1 Thermodynamic Version of Wick's Theorem 393
- Appendix 5A Liénard-Wiechert Potential 398
- Appendix 5B Equal-Time Commutator from Time-Ordered Product . . 399
- Appendix 5C Euler-Maclaurin formula 401
- Notes and References 405

6 Continuous Symmetries and Conservation Laws; Noether's Theorem 406
- 6.1 Point Mechanics 406
  - 6.1.1 Continuous Symmetries and Conservation Law 406
  - 6.1.2 Alternative Derivation 408
- 6.2 Displacement and Energy Conservation 410
- 6.3 Momentum and Angular Momentum 411
  - 6.3.1 Center-of-Mass Theorem 413
  - 6.3.2 Conservation Laws from Lorentz Invariance 415
- 6.4 Generating the Symmetries 417
- 6.5 Field Theory 418
  - 6.5.1 Continuous Symmetry and Conserved Currents 419
  - 6.5.2 Alternative Derivation 420
- 6.6 Canonical Energy Momentum Tensor 421
  - 6.6.1 Electromagnetism 423
  - 6.6.2 Dirac Field 424
- 6.7 Angular Momentum 425
- 6.8 Four-Dimensional Angular Momentum 426
- 6.9 Spin Current 428
  - 6.9.1 Electromagnetic Fields 428
  - 6.9.2 Dirac Field 431

6.10 Symmetric Energy Momentum Tensor . . . 432
6.11 Internal Symmetries . . . 434
  6.11.1 U(1)-Symmetry and Charge Conservation . . . 435
  6.11.2 SU(N)-Symmetry . . . 436
  6.11.3 Broken Internal Symmetries . . . 436
6.12 Generating the Symmetry Transformations on Quantum Fields . . . 436
6.13 Energy Momentum Tensor of a Relativistic Massive Point Particle . 438
6.14 Energy Momentum Tensor of Charged Particles in an Electromagnetic Field . . . 439
Notes and References . . . 442

7 Scattering and Decay of Particles 443
7.1 INTERACTION PICTURE . . . 443
7.2 DISCRETE STATES . . . 450
7.3 Scattering Amplitude . . . 456
  7.3.1 Center-of-Mass Scattering Cross Section . . . 469
  7.3.2 Laboratory Scattering Cross Section . . . 471
7.4 DECAY . . . 474
7.5 OPTICAL THEOREM . . . 474
7.6 INITIAL- AND FINAL-STATE INTERACTIONS . . . 475
7.7 TESTS OF TIME-REVERSAL VIOLATIONS . . . 477
  7.7.1 Strong and Electromagnetic Interactions . . . 477
  7.7.2 Selection Rules in Weak Interactions . . . 478
  7.7.3 Phase of Weak Amplitudes from Time-Reversal Invariance 479
Notes and References . . . 480

8 Quantum Field Theoretic Perturbation Theory 481
8.1 The Interacting n-Point Function . . . 481
8.2 Perturbation Expansion for Green Functions . . . 483
8.3 Feynman Rules for ϕ^4-theory . . . 485
  8.3.1 The Vacuum Graphs . . . 487
8.4 The Two-Point Function . . . 489
8.5 The Four-Point Function . . . 491
8.6 Connected Green Function . . . 493
  8.6.1 One-Particle Irreducible Graphs . . . 497
  8.6.2 Momentum Space Version of Diagrams . . . 499
8.7 Green Functions and Scattering Amplitudes . . . 502
8.8 Wick Rules for Scattering Amplitudes . . . 508
8.9 Thermal Perturbation Theory . . . 509

9 Extracting Finite Results from Perturbation Series. Regularization and Renormalization 513
9.1 Vacuum Diagrams . . . 513
9.2 The Two- and Four-Point Functions . . . 516

9.3 Divergences, Cutoff, and Counterterms 518
9.4 Bare Theory and Multiplicative Renormalization 525
9.5 Dimensional Regularization of Integrals 529
9.6 Renormalization of Amplitudes 543
9.7 Generalization to O(N)-Symmetric Model 546
9.8 Finite S-Matrix Elements 551
Appendix 9A Alternative Proof of Veltman's Integral Rule 553
Notes and References 555

10 Quantum Electrodynamics 556
10.1 Gauge Invariant Interacting Theory 556
  10.1.1 Reminder of Classical Electrodynamics of Point Particles . . 557
  10.1.2 Electrodynamics and Quantum Mechanics 559
  10.1.3 Electrodynamics and Relativistic Quantum Mechanics . . . 561
10.2 Noether's Theorem and Gauge Fields 563
10.3 Quantization 564
10.4 Perturbation Theory 568
10.5 Magnetic Moment of Electron 572
10.6 Decay of Atomic State 575
10.7 Rutherford Scattering 582
  10.7.1 Classical Cross Section 582
  10.7.2 Quantum-Mechanical Born Approximation 583
  10.7.3 Relativistic Born Approximation 584
10.8 Compton Scattering 587
  10.8.1 Classical Result 588
  10.8.2 Klein-Nishina Formula 589
10.9 Electron-Positron Annihilation 595

10 Functional Integral Representation of Quantum Field Theory 556
10.1 Functional Fourier Transform 556
10.2 Gaussian Functional Integral 557
10.3 Functional Definition of Free Quantum Field Theories 561
10.4 Interactions 562
10.5 Euclidean Quantum Field Theory 565
10.6 Functional Integral Representation for Fermions 566
10.7 Relation Between $Z[j]$ and Partition Function 569
10.8 Bosons and Fermions in a Single State 574
10.9 Free Energy for Free Scalar Fields 576
10.10 Gauge Fields and Gauge Fixing 577
10.11 Nontrivial Gauge and Fadeev-Popov Ghosts 584

12 Formal Properties of Perturbation Theory 644
12.1 Connectedness Structure of Feynman Diagrams 644
12.2 Functional Differential Equations 645

12.3 Decomposition of Green Functions into Connected Green Functions 647
12.4 Functional Differential Equation for $W[j[$ 649
12.5 Iterative Solution 649
12.6 Vertex Functions 651
12.7 The Generating Functional for Vertex Functions 651
12.8 Functional Differential Equation for $\Gamma[\Phi]$ 657
12.9 Effective Action as a Basis for Variational Calculations 660
12.10 Effective Potential 660

13 Systematic Graphical Construction of Feynman Diagrams . . . 662
13.1 Generalized Scalar ϕ^4-Theory 663
13.2 Basic Graphical Operations 665
  13.2.1 Cutting Lines 665
  13.2.2 Removing Lines 668
13.3 Perturbation Theory 669
13.4 Functional Differential Equation for $W = \ln Z$ 670
13.5 Recursion Relation and Graphical Solution 672
13.6 Scalar $\phi^2 A$-Theory 674
13.7 Perturbation Theory 676
13.8 Functional Differential Equation for $W = \ln Z$ 676
13.9 Recursion Relation and Graphical Solution 677
13.10 Computer Generation of Diagrams 679
13.11 Matrix Representation of Diagrams 679
13.12 Practical Generation 681
  13.12.1 Connected Vacuum Diagrams 681
  13.12.2 Two- and Four-Point Functions $\mathbf{G}_{12}$ and $\mathbf{G}^c_{1234}$ from Cutting Lines 684
  13.12.3 Two- and Four-Point Function $\mathbf{G}_{12}$ and $\mathbf{G}^c_{1234}$ from Removing Lines 685

14 Path Integral Calculation of Effective Action. Loop Expansion 696
14.1 General Formalism 696
14.2 Quadratic Fluctuations 699
14.3 Massless Theory 703
14.4 Effective Action to Second Order in $\hbar$ 706
14.5 Effective Action to all Orders in $\hbar$ 710

15 Spontaneous Symmetry Breakdown 713
15.1 Scalar O(N)-Symmetric ϕ^4-Theory 713
15.2 Nambu-Goldstone Particles 719
  15.2.1 The Mechanism 719
  15.2.2 General Considerations 721
  15.2.3 Experimental Consequences 722
15.3 Domain Walls in O(1)-Symmetric Theory 724

15.4 Vortex Lines in O(2)-Symmetric Theory 729

1 Scalar Quantum Electrodynamics 1
1.1 Action and Generating Functional 1
1.2 Meissner-Higgs Effect 4
1.3 Spatially Varying Ground States 10
1.4 Two Natural Length Scales 11
1.5 Planar Domain Wall 13
1.6 Surface Energy 19
1.7 Single Vortex Line and Critical Field H_{c1} 20
1.8 Critical Field H_{c2} where Superconductivity is Destroyed 26

15 Exactly Solvable O(N)-Symmetric ϕ^4-Theory for Large N 713
15.1 Introduction of a Collective Field 713
15.2 The Limit of Large N 716
15.3 Variational Equations 723
  15.3.1 Non-trivial Ground States 724
15.4 Special Features of Two Dimensions 728
15.5 Experimental Consequences 730
15.6 Correlation Functions for Large N 733

16 Non-Linear σ-Model 737
16.1 Definition of Classical Heisenberg Model 737
16.2 Spherical Model 740
16.3 Free Energy and Gap Equation in $D > 2$ Dimensions 741
  16.3.1 High-Temperature Phase 743
  16.3.2 Low-Temperature Phase 744
16.4 Approaching the Critical Point 746
16.5 Physical Property of Bare Temperature 747
16.6 Spherical Model on Lattice 749
16.7 Background Field Treatment of Cold Phase 753
16.8 Quantum Statistics at Nonzero Temperature Nonlinear σ-Model in D Spacetime Dimensions 755
  16.8.1 Two-Dimensional Model 755
  16.8.2 Four-Dimensional Model 760
  16.8.3 Any Dimension 761
16.9 Criteria for Onset of Fluctuations in Ginzburg-Landau Theories . . . 766
  16.9.1 Ginzburg's Criterion 767
  16.9.2 Kleinert's Criterion 768
  16.9.3 Experimental Consequences 770

17 Phase Transitions in Hydrodynamic Limit 773
17.1 Goldstone Modes with Line-like Topological Defects 774
17.2 Superfluid ^{4}He 778
  17.2.1 Gradient Energy 778

17.2.2 Vortex Density 779
17.2.3 Partition Function 780
17.2.4 Interaction Energy between Vortices 781
17.2.5 Kosterlitz-Thouless Transition in Films of Superfluid Helium 781
17.2.6 Physical Jumping Surfaces 783
17.2.7 Gauge Field of Superflow 784
17.2.8 Disorder Field Theory 786
17.2.9 Disorder Theory of Superconductor 789
17.2.10 Order versus Disorder 792
17.2.11 Order of Superconducting Phase Transition and Tricritical Point 797
17.2.12 Vortex Lattices 797
17.3 Crystals 799
17.4 Charge Confinement 805
Notes and References 808

18 Exactly Solvable O(N)-Symmetric Four-Fermion Theory in $2+\epsilon$ Dimensions 809
18.1 Scalar Self-Interaction 809
18.2 Spontanous Symmetry Breakdown 814
18.3 Dimensionally Transmuted Coupling Constant 815
18.4 Scattering Amplitude for Fermions 816
18.5 Nonzero Bare Fermion Mass 823
18.6 Pairing Model and Dynamically Generated Goldstone Bosons 824
18.7 Spontanously Broken Symmetry 832
18.8 Relation between Pairing and Gross-Neveu Model 835
18.9 Comparison with O(N)-Symmetric ϕ^4-Theory 836
18.10 Two Phase Transitions in Chiral Gross-Neveu Model 841
18.11 Finite-Temperature Properties 844
Notes and References 855

19 The Renormalization Group 857
19.1 Example for Redundancy in Parametrization of Renormalized Theory 858
19.2 Renormalization Scheme 860
19.3 The Renormalization Group Equation 862
19.4 Calculation of Coefficient Functions from Counter Terms 863
19.5 Solution of Renormalization Group Equations for Vertex Functions . 867
19.6 Renormalization Group for Effective Action and Potential 871
19.7 Approach to Scaling 873
19.8 Explicit Solution of the RGE close to $D=4$ Dimensions 875
19.9 Further Critical Relations 879
19.9.1 Scaling Relations Above T_c 879
19.9.2 Scaling Relations Below T_c 881
19.10 Comparison of Scaling Relations with Experiment 883

19.11 Higher-Order Expansion 885
19.12 Mean-Field Results for Critical Indices 886
19.13 Effective Potential in the Critical Regime to Order ϵ 889
19.14 O(N)-Symmetric Theory 894
19.15 Direct Scaling Form in the Limit of Large $N \to \infty$ 897

20 Internal Symmetries of Strong Interactions 898
20.1 Classification of Elementary Particles 898
20.2 Isospin in Nuclear Physics 901
20.3 Isospin in Pion Physics 906
20.4 SU(3)-Symmetry 909
20.5 New Quarks 929
20.6 Tensor Representations and Young Tableaux 929
20.7 Effective Interactions among Hadrons 934
  20.7.1 The Pion-Nucleon Interaction 934
  20.7.2 The Decay $\Delta(1232) \to N\pi$ 937
  20.7.3 The Vector Meson Decay $\rho(770) \to \pi\pi$ 942
  20.7.4 The Axial Vector Meson Decay $a_1(1270) \to \rho\pi$ 944
Appendix 20A Useful SU(3) Formulas 946
Appendix 20B Decay rate for $a_1 \to \rho\pi$ 949

21 Symmetries Linking Internal and Spacetime Structure 951
21.1 Approximate SU(4)-Symmetry of Nuclear Forces 951
21.2 SU(6) Symmetry of Strong Interactions 959
21.3 SU(6) and Current Algebra 966
21.4 Supersymmetry 971

22 Quantum Field Theory of Elementary Particles 975
22.1 Electromagnetism 976
22.2 Gravity 978
22.3 Strong Interactions 979
22.4 Weak Interactions 984
Notes and References 995

23 Critical Properties of Non-linear σ-Model 996
23.1 INTRODUCTORY REMARKS 996
23.2 PERTURBATION THEORY 998
23.3 SYMMETRY PROPERTIES OF RENORMALIZED EFFECTIVE ACTION 1003
23.4 CRITICAL BEHAVIOUR IN $2+\epsilon$ DIMENSIONS 1006
23.5 CRITICAL EXPONENTS 1007
23.6 TWO- AND THREE-LOOP RESULTS 1014
23.7 VARIATIONAL RESUMMATION OF ϵ-EXPANSIONS 1017
  23.7.1 Strong-Coupling Theory 1019
  23.7.2 Interpolation 1022

23.8 RELATION BETWEEN σ-MODEL AND QUANTUM MECHANICS OF POINT PARTICLE ON SPHERE 1025
23.9 GENERALIZATION OF MODEL 1035
Notes and References 1037

List of Figures

List of Tables

1

Fundamentals

Before turning to the actual subject of this text it is useful to recall some of the theoretical background underlying the theory to be developed.

1.1 Quantum Mechanics

Historically, the extension of classical mechanics to quantum mechanics became necessary in order to understand the stability of atomic orbits and the discrete nature of atomic spectra. It soon became clear that these phenomena reflect the fact that at a sufficiently short length scale, small material particles such as electrons behave like waves, called *material waves*. The fact that waves cannot be squeezed into an arbitrarily small volume without increasing indefinitely their frequency and thus their energy, prevents the collapse of the electrons into the nucleus, which would take place in classical mechanics. The discreteness of the atomic states of an electron are a manifestation of standing material waves in the atomic potential well, in analogy with the standing waves of electromagnetism in a cavity.

The most direct manifestation of the wave nature of small particles is seen in diffraction experiments on periodic structures, for example of electrons diffracted by a crystal. If an electron beam of fixed momentum $\mathbf{p}$ passes through a crystal, it emerges along sharply peaked angles. These are the well-known *Bragg reflections*. They look very similar to the interference patterns of electromagnetic waves. In fact, it is possible to use the same mathematical framework to explain these patterns as in electromagnetism. A free particle of a given momentum $\mathbf{p}$ is described by a field strength or *wave function*

$$\Psi_{\mathbf{p}}(\mathbf{x},t) = e^{i\mathbf{kx}-i\omega t}, \tag{1.1}$$

where $\mathbf{k}$ is the *wave vector* pointing into the direction of $\mathbf{p}$ and ω is the *wave frequency*. Each scattering center, say at $\mathbf{x}'$, becomes a source of a spherical wave with the spatial behavior e^{ikR}/R (with $R \equiv |\mathbf{x}-\mathbf{x}'|$ and $k \equiv |\mathbf{k}|$) and the wavelength $\lambda = 2\pi/k$. At the detector, all field strengths have to be added to the total field strength $\Psi(\mathbf{x},t)$. The absolute square of the total field strength, $|\Psi(\mathbf{x},t)|^2$, is proportional to the number of electrons arriving at the detector.

The standard experiment where these rules can most simply be applied consists of an electron beam impinging vertically upon a flat screen with two parallel slits a distance d apart. Behind these, one observes the number of particles arriving per unit time (see Fig. 1.1)

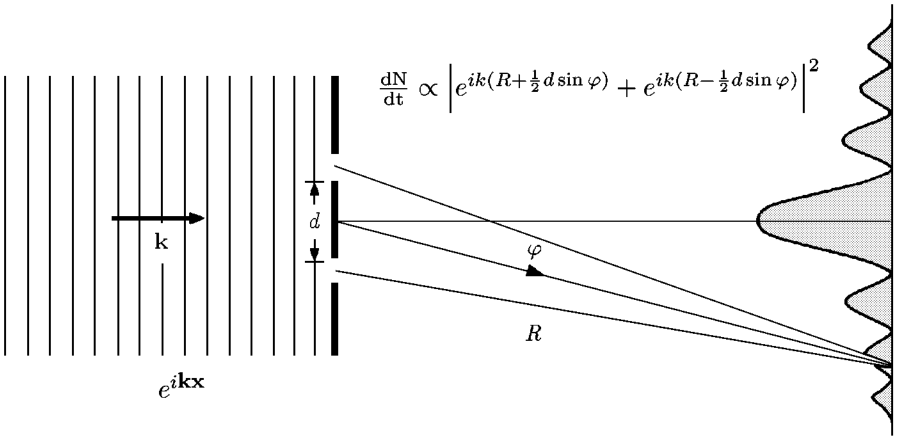
$\frac{\mathrm{dN}}{\mathrm{dt}} \propto \left| e^{ik(R+\frac{1}{2}d\sin\varphi)} + e^{ik(R-\frac{1}{2}d\sin\varphi)} \right|^2$
k
d
φ
R
$e^{i\mathbf{kx}}$

FIGURE 1.1 Probability distribution of particle behind a double slit, being proportional to the absolute square of the sum of the two complex field strengths.

$$\frac{dN}{dt} \propto |\Psi_1 + \Psi_2|^2 \approx \left| e^{ik(R+\frac{1}{2}d\sin\varphi)} + e^{ik(R-\frac{1}{2}d\sin\varphi)} \right|^2 \frac{1}{R^2}. \tag{1.2}$$

where φ is the angle of deflection from the normal.

Conventionally, the wave function $\psi(\mathbf{x}, t)$ is normalized to describe a single particle. Its absolute square

$$\rho(\mathbf{x}, t) = \psi^*(\mathbf{x}, t)\psi(\mathbf{x}, t) \tag{1.3}$$

gives directly the *probability density* for finding the particle at the place $\mathbf{x}$ in space, i.e. $d^3x\ |\psi(\mathbf{x}, t)|^2$ is the probability that the particle is found in the volume element d^3x around $\mathbf{x}$.

From the experimentally observed relation between the momentum and the size of the angular deflection φ of the diffracted beam of the particles, one deduces the relation between momentum and wave vector

$$\mathbf{p} = \hbar\mathbf{k}, \tag{1.4}$$

where $\hbar$ is a universal constant whose dimension is equal to that of an action,

$$\hbar \equiv \frac{h}{2\pi} = 1.0545919(80) \times 10^{-27}\mathrm{erg\,sec} \tag{1.5}$$

(the number in parentheses indicating the experimental uncertainty of the last two digits before it). A similar relation holds between the energy and the frequency of the wave $\Psi(\mathbf{x}, t)$. It may be determined by an absorption process in which a light wave hits an electron (for example, by kicking it out of the surface of a metal, the well-known *photoeffect*). From the threshold property of the photoeffect one learns that an electromagnetic wave oscillating in time as $e^{-i\omega t}$ can transfer to the electron the energy

$$E = \hbar\omega, \tag{1.6}$$

where the proportionality constant $\hbar$ is the same as in (1.4). The reason for this lies in the properties of electromagnetic waves. On the one hand, their frequency ω and the wave vector $\mathbf{k}$ satisfy the relation $\omega/c = |\mathbf{k}|$, where c is the light velocity. On the other hand, energy and momentum are related by $E/c = |\mathbf{p}|$. Thus, the quanta of electromagnetic waves, the *photons*, certainly satisfy (1.4) and the constant $\hbar$ must be the same as in Eq. (1.6).

With matter waves and photons sharing the same relations (1.4), it is suggestive to postulate also the relation (1.6) between energy and frequency to be universal for the waves of all particles, massive and massless ones. A free particle with momentum $\mathbf{p}$ is described by a *plane wave* of wavelength $\lambda = 2\pi/|\mathbf{k}| = 2\pi\hbar/|\mathbf{p}|$, with the explicit form

$$\Psi_{\mathbf{p}}(\mathbf{x}, t) = \mathcal{N} e^{i(\mathbf{p}\mathbf{x} - E_{\mathbf{p}}t)/\hbar}, \tag{1.7}$$

where $\mathcal{N}$ is some normalization constant. In a finite volume, the wave function is normalized to unity. In an infinite volume, this normalization makes the wave function vanish. To avoid this, the current density is normalized to unity. The energy $E_{\mathbf{p}}$ depends on the momentum of the particle in the classical way, i.e., for nonrelativistic material particles of mass M it is $E_{\mathbf{p}} = \mathbf{p}^2/2M$, for relativistic ones $E_{\mathbf{p}} = c\sqrt{\mathbf{p}^2 + M^2c^2}$, and for massless particles such as photons $E_{\mathbf{p}} = c|\mathbf{p}|$. The common relation $E_{\mathbf{p}} = \hbar\omega$ for photons and matter waves is necessary to guarantee conservation of energy in quantum mechanics.

In general, momentum and energy of a particle are not defined as well as in the plane-wave function (1.7). Usually, a particle wave is some superposition of plane waves (1.7)

$$\Psi(\mathbf{x}, t) = \int \frac{d^3p}{(2\pi\hbar)^3} f(\mathbf{p}) e^{i(\mathbf{p}\mathbf{x} - E_{\mathbf{p}}t)/\hbar}. \tag{1.8}$$

By the Fourier inversion theorem, $f(\mathbf{p})$ can be calculated via the integral

$$f(\mathbf{p}) = \int d^3x \, e^{-i\mathbf{p}\mathbf{x}/\hbar} \Psi(\mathbf{x}, 0). \tag{1.9}$$

With an appropriate choice of $f(\mathbf{p})$ it is possible to prepare $\Psi(\mathbf{x}, t)$ in any desired form at some initial time, say at $t = 0$. For example, $\Psi(\mathbf{x}, 0)$ may be a function sharply centered around a space point $\bar{\mathbf{x}}$. Then $f(\mathbf{p})$ is approximately a pure phase $f(\mathbf{p}) \sim e^{-i\mathbf{p}\bar{\mathbf{x}}/\hbar}$, and the wave contains all momenta with equal probability. Conversely, if the particle amplitude is spread out in space, its momentum distribution is confined to a small region. The limiting $f(\mathbf{p})$ is concentrated at a specific momentum $\bar{\mathbf{p}}$. The particle is found at each point in space with equal probability, with the amplitude oscillating like $\Psi(\mathbf{x}, t) \sim e^{i(\bar{\mathbf{p}}\mathbf{x} - E_{\bar{\mathbf{p}}}t)/\hbar}$.

In general, the width of $\Psi(\mathbf{x}, 0)$ in space and of $f(\mathbf{p})$ in momentum space are inversely proportional to each other:

$$\Delta\mathbf{x}\,\Delta\mathbf{p} \sim \hbar. \tag{1.10}$$

This is the content of *Heisenberg's principle of uncertainty*. If the wave is localized in a finite region of space while having at the same time a fairly well-defined average momentum $\bar{\mathbf{p}}$, it is called a *wave packet*. The maximum in the associated probability density can be shown from (1.8) to move with a velocity

$$\bar{\mathbf{v}} = \partial E_{\bar{\mathbf{p}}}/\partial \bar{\mathbf{p}}. \tag{1.11}$$

This coincides with the velocity of a classical particle of momentum $\bar{\mathbf{p}}$.

Suppose now that the particle is nonrelativistic and has a mass M. The classical Hamiltonian, and thus the energy $E_{\mathbf{p}}$, are given by

$$H(\mathbf{p}) = E_{\mathbf{p}} = \frac{\mathbf{p}^2}{2M}. \tag{1.12}$$

We may therefore derive the following identity for the wave field $\Psi_{\mathbf{p}}(\mathbf{x},t)$:

$$\int \frac{d^3p}{(2\pi\hbar)^3} f(\mathbf{p}) \left[H(\mathbf{p}) - E_{\mathbf{p}}\right] e^{i(\mathbf{p}\mathbf{x}-E_{\mathbf{p}}t)/\hbar} = 0. \tag{1.13}$$

The arguments *inside* the brackets can be removed from the integral by observing that $\mathbf{p}$ and $E_{\mathbf{p}}$ inside the integral are equivalent to the differential operators

$$\begin{aligned} \hat{\mathbf{p}} &= -i\hbar\partial_{\mathbf{x}}, & (1.14)\\ \hat{E} &= i\hbar\partial_t & (1.15) \end{aligned}$$

outside. Then, Eq. (1.13) may be written as the differential equation

$$[H(-i\hbar\partial_{\mathbf{x}}) - i\hbar\partial_t)]\Psi(\mathbf{x},t) = 0. \tag{1.16}$$

This is the *Schrödinger equation* for the wave function of a free particle. The equation suggests that the motion of a particle with an arbitrary Hamiltonian $H(\mathbf{p},\mathbf{x},t)$ follows the straightforward generalization of (1.16)

$$\left(\hat{H} - i\hbar\partial_t\right)\Psi(\mathbf{x},t) = 0, \tag{1.17}$$

where $\hat{H}$ is the differential operator

$$\hat{H} \equiv H(-i\hbar\partial_{\mathbf{x}}, \mathbf{x}, t). \tag{1.18}$$

The rule of obtaining $\hat{H}$ from the classical Hamiltonian $H(\mathbf{p},\mathbf{x},t)$ by the substitution $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\partial_{\mathbf{x}}$ will be referred to as the *correspondence principle*.

It is important to emphasize that this simple form of the correspondence principle holds initially only for Cartesian coordinates.[1] Only a slight generalization is possible to generalized coordinates $q_i(t)$ which are of the *quasi-Cartesian* type. For these, the so-called *dynamical metric*, or *Hessian*), defined in the Lagrangian formalism by

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[1] For details see the textbook H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics, World Scientific, Singapore, 1995. The substitution rule for the momentum runs also under the name *Jordan rule*.

$$g_{ij}(q) \equiv \frac{\partial^2}{\partial \dot{q}_i \partial \dot{q}_i} L(q, \dot{q}), \tag{1.19}$$

and in the Hamiltonain formalism by

$$g^{ij}(q) \equiv \frac{\partial^2}{\partial p_i \partial p_j} H(p, q), \tag{1.20}$$

must be q_i-independent and proportional to the unit matrix. Then the momentum operators are, as in (1.14),

$$\hat{p}_i \equiv -i \frac{\hat{\partial}}{\partial q_i}. \tag{1.21}$$

For such quasi-Cartesian generalized coordinates, the system may be quantized alternatively à la Heisenberg by assuming $p_i(t)$ and $q_i(t)$ to be Heisenberg operators $\hat{p}_{i\,\mathrm{H}}(t)$ and $\hat{q}_{i\,\mathrm{H}}(t)$ satisfying the canonical commutation rules (1.237):

$$\begin{aligned} \left[\hat{p}_{i\mathrm{H}}(t), \hat{q}_{j\mathrm{H}}(t)\right] &= -i\hbar\delta_{ij}, \\ \left[\hat{p}_{i\mathrm{H}}(t), \hat{p}_{j\mathrm{H}}(t)\right] &= 0, \\ \left[\hat{q}_{i\mathrm{H}}(t), \hat{q}_{j\mathrm{H}}(t)\right] &= 0. \end{aligned} \tag{1.22}$$

The validity of the Schrödinger equation (1.17) is confirmed by experiment, most notably for the Coulomb Hamiltonian

$$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2M} - \frac{e^2}{r}, \tag{1.23}$$

which governs the quantum mechanics of the hydrogen atom in the center-of-mass coordinate system of electron and proton, where M is the reduced mass of the two particles.

Since the square of the wave function, $|\Psi(\mathbf{x}, t)|^2$, is interpreted as the probability density of a single particle in a finite volume, the integral over the entire volume must be normalized to unity:

$$\int d^3x \, |\Psi(\mathbf{x}, t)|^2 = 1. \tag{1.24}$$

For a stable particle, this normalization must remain the same at all times. If $\Psi(\mathbf{x}, t)$ is to follow the Schrödinger equation (1.17), this is assured if and only if the Hamilton operator is Hermitian,[2] i.e., if it satisfies for arbitrary wave functions Ψ_1, Ψ_2 the equality

$$\int d^3x\, [\hat{H}\Psi_2(\mathbf{x},t)]^*\Psi_1(\mathbf{x},t) = \int d^3x\, \Psi_2^*(\mathbf{x},t)\hat{H}\Psi_1(\mathbf{x},t). \tag{1.25}$$

The left-hand side defines the *Hermitian-adjoint* $\hat{H}^\dagger$ of the operator $\hat{H}$, having for all states $\Psi_1(\mathbf{x},t), \Psi_2(\mathbf{x},t)$:

$$\int d^3x\, \Psi_2^*(\mathbf{x},t)\hat{H}^\dagger\Psi_1(\mathbf{x},t) \equiv \int d^3x\, [\hat{H}\Psi_2(\mathbf{x},t)]^*\Psi_1(\mathbf{x},t). \tag{1.26}$$

An operator $\hat{H}$ is *Hermitian*, if it coincides with its Hermitian-adjoint $\hat{H}^\dagger$:

$$H = H^\dagger.$$

Let us calculate the time change of the integral over two arbitrary wave functions, $\int d^3x\, \Psi_2^*(\mathbf{x},t)\Psi_1(\mathbf{x},t)$. With the Schrödinger equation (1.17), this time change vanishes indeed as long as $\hat{H}$ is Hermitian:

$$\begin{aligned} i\hbar\frac{d}{dt}&\int d^3x\, \Psi_2^*(\mathbf{x},t)\Psi_1(\mathbf{x},t) \\ = &\int d^3x\, \Psi_2^*(\mathbf{x},t)\hat{H}\Psi_1(\mathbf{x},t) - \int d^3x\, [\hat{H}\Psi_2(\mathbf{x},t)]^*\Psi_1(\mathbf{x},t) = 0. \end{aligned} \tag{1.27}$$

This also implies the time independence of the normalization integral $\int d^3x\, |\Psi(\mathbf{x},t)|^2 = 1$.

Conversely, if $\hat{H}$ is not Hermitian, one can always find an eigenstate of $\hat{H}$ whose norm changes with time: any eigenstate of $(H - H^\dagger)/i$ has this property.

Since $\hat{\mathbf{p}} = -i\hbar\partial_{\mathbf{x}}$ and $\mathbf{x}$ are themselves Hermitian operators, $\hat{H}$ will automatically be a Hermitian operator if it is a sum of a kinetic and a potential energy:

$$H(\mathbf{p},\mathbf{x},t) = T(\mathbf{p},t) + V(\mathbf{x},t). \tag{1.28}$$

This is always the case for nonrelativistic particles in Cartesian coordinates $\mathbf{x}$. If $\mathbf{p}$ and $\mathbf{x}$ appear in one and the same term of H, for instance as $\mathbf{p}^2\mathbf{x}^2$, the correspondence principle does not lead to a unique quantum-mechanical operator $\hat{H}$. Then there seem to be, in principle, several Hermitian operators which, in the above example, can be constructed from the product of two $\hat{\mathbf{p}}$ and two $\hat{\mathbf{x}}$ operators [for instance $\alpha\hat{\mathbf{p}}^2\hat{\mathbf{x}}^2 + \beta\hat{\mathbf{x}}^2\hat{\mathbf{p}}^2 + \gamma\hat{\mathbf{p}}\hat{\mathbf{x}}^2\hat{\mathbf{p}}$ with $\alpha + \beta + \gamma = 1$]. They all correspond to the same classical $\mathbf{p}^2\mathbf{x}^2$. At first sight it appears as though only a comparison with experiment could select the correct operator ordering. This is referred to as the operator-ordering problem of *quantum mechanics* which has plagued many researchers in the past. For a large class of systems, this problem is caused by a nontrivial geometry of spacetime. In that case the problem has recently found a surprisingly simple solution.[3] In the present text we shall generally be able to avoid operator-ordering ambiguities, since our Hamiltonian $H(\mathbf{p},\mathbf{x},t)$ will always have the form (1.28), with only one exception, the nonlinear σ-model in Chapter 18.

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[2] Problems arising from unboundedness or discontinuities of the Hamiltonian and other quantum-mechanical operators, such as restrictions of the domains of definition, are ignored here since they are well understood. Correspondingly we do not distinguish between Hermitian and self-adjoint operators (see J. v. Neumann, *Mathematische Grundlagen der Quantenmechanik*, Springer, Berlin, 1932). Some quantum-mechanical operator subtleties will manifest themselves in this book as problems of path integration to be solved in Chapter 12. The precise relationship between the two calls for further detailed investigations.

The conservation of the total probability (1.24) is a consequence of a more general local conservation law linking the *current density* of the particle probability

$$\mathbf{j}(\mathbf{x},t) \equiv -i\frac{\hbar}{2m}\psi^*(\mathbf{x},t)\overleftrightarrow{\boldsymbol{\nabla}}\psi(\mathbf{x},t) \tag{1.29}$$

with the probability density (1.3) via the relation

$$\partial_t\rho(\mathbf{x},t) = -\boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{x},t). \tag{1.30}$$

In (1.29) we have used the standard quantum-mechanical notation that $\overleftrightarrow{\boldsymbol{\nabla}}$ denotes the difference beteen right- and left-derivatuves

$$\begin{aligned}\psi^*(\mathbf{x},t)\overleftrightarrow{\boldsymbol{\nabla}}\psi(\mathbf{x},t) &\equiv \psi^*(\mathbf{x},t)\overrightarrow{\boldsymbol{\nabla}}\psi(\mathbf{x},t) - \psi^*(\mathbf{x},t)\overleftarrow{\boldsymbol{\nabla}}\psi(\mathbf{x},t)\\ &\equiv \psi^*(\mathbf{x},t)\boldsymbol{\nabla}\psi(\mathbf{x},t) - [\boldsymbol{\nabla}\psi^*(\mathbf{x},t)]\,\psi(\mathbf{x},t).\end{aligned} \tag{1.31}$$

The energy $E_\mathbf{p}$ depends By integrating this *current conservation law* over a volume V enclosed by a surface S, and using the Gauss theorem, one finds

$$\int_V d^3x\,\partial_t\rho(\mathbf{x},t) = -\int_V d^3x\,\boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{x},t) = -\int_S d\mathbf{S}\cdot\mathbf{j}(\mathbf{x},t) \tag{1.32}$$

where $d\mathbf{S}$ are the directed infinitesimal surface elements. This equation states that the probability in a volume decreases by the same amount by which probability leaves the surface via the current $\mathbf{j}(\mathbf{x},t)$.

By extending the integral over the entire space and assuming the currents to vanish at spatial infinity, we recover the conservation of the total probability (1.24).

In Chapters 3 and 5 we shall find relativistic versions of this conservation law. These will be extended in Chapter 6 by a wide variety of further local conservation laws, where we shall learn that all of them are closely linked to certain symmetry properties of the systems.

The more general dynamical system with N particles in euclidean space, is parametrized in terms of $3N$ Cartesian coordinates $\mathbf{x}_\nu(\nu = 1,\dots,N)$, the Hamiltonian has the form

$$H(\mathbf{p}_\nu,\mathbf{x}_\nu,t) = \sum_{\nu=1}^{N}\frac{\mathbf{p}_\nu^2}{2M_\nu} + V(\mathbf{x}_\nu,t), \tag{1.33}$$

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[3] See the textbook in Footnote 1

where the arguments $\mathbf{p}_\nu, \mathbf{x}_\nu$ in H and V stand for all $\mathbf{p}_\nu$'s, $\mathbf{x}_\nu$'s. The components of $\mathbf{x}_\nu$ all range from $-\infty$ to ∞. The wave function $\psi(\mathbf{x}_\nu, t)$ satisfies the N-particle Schrödinger equation,

$$\left[-\sum_{\nu=1}^{N} \frac{\hbar^2}{2M_\nu} \partial_{\mathbf{x}_\nu}{}^2 + V(\mathbf{x}_\nu, t)\right] \psi(\mathbf{x}_\nu, t) = i\hbar\partial_t \psi(\mathbf{x}_\nu, t). \tag{1.34}$$

1.2 Dirac's Bra-Ket Formalism

Mathematically speaking, the wave function $\Psi(\mathbf{x}, t)$ may be considered as a vector in an infinite-dimensional complex vector space called the *Hilbert space*. The configuration space variable $\mathbf{x}$ plays the role of a continuous "index" of these vectors. An obvious contact with the usual vector notation may be established, in which a D-dimensional vector $\mathbf{v}$ is given in terms of its components v_i with a subscript $i = 1, \ldots D$, by writing the argument $\mathbf{x}$ of $\Psi(\mathbf{x}, t)$ as a subscript:

$$\Psi(\mathbf{x}, t) \equiv \Psi_{\mathbf{x}}(t). \tag{1.35}$$

The usual norm of a complex vector is defined by

$$|\mathbf{v}|^2 = \sum_i v_i^* v_i. \tag{1.36}$$

The continuous version of this is

$$|\Psi|^2 = \int d^3x \, \Psi_{\mathbf{x}}^*(t) \Psi_{\mathbf{x}}(t) = \int d^3x \, \Psi^*(\mathbf{x}, t) \Psi(\mathbf{x}, t). \tag{1.37}$$

The normalization condition (1.24) requires that the wave functions have the norm $|\Psi| = 1$, i.e., that they are unit vectors in the Hilbert space.

In a vector space, there are many possible choices of orthonormal basis vectors $b_i{}^a$ labeled by $a = 1, \ldots, D$, in terms of which[4]

$$v_i = \sum_a b_i{}^a v_a, \tag{1.38}$$

with the components v_a given by the scalar products

$$v_a \equiv \sum_i b_i{}^{a*} v_i. \tag{1.39}$$

The latter equation is a consequence of the orthonormality relation

$$\sum_i b_i{}^{a*} b_i{}^{a'} = \delta^{aa'}, \tag{1.40}$$

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[4] Mathematicians would expand more precisely $v_i = \sum_a b_i{}^a v_a^{(b)}$, but physicists prefer to shorten the notation by distinguishing the different components via different types of subscripts, using for the initial components $i, j, k, \ldots$ and for the b-transformed components $a, b, c, \ldots$.

which in a finite-dimensional vector space implies the completeness relation

Similarly, there are many possible orthonormal basis functions $f^a(\mathbf{x})$ in the Hilbert space which satisfy the orthogonality relation

$$\int d^3x\, f^a(\mathbf{x})^* f^{a'}(\mathbf{x}) = \delta^{aa'}, \tag{1.41}$$

and the completeness relation [which is here not automatically implied by (1.154)]

$$\sum_a f^a(\mathbf{x}) f^a(\mathbf{x})^* = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{1.42}$$

thus serving to expand

$$\Psi(\mathbf{x},t) = \sum_a f^a(\mathbf{x}) \Psi_a(t), \tag{1.43}$$

with the coefficients

$$\Psi_a(t) = \int d^3x\, f^a(\mathbf{x})^*\, \Psi(\mathbf{x},t). \tag{1.44}$$

Certainly, one may use any other orthonormal basis $\tilde{f}^b(\mathbf{x})$ with the orthogonality and completeness relations

$$\int d^3x\, \tilde{f}^b(\mathbf{x})^* \tilde{f}^{b'}(\mathbf{x}) = \delta^{bb'}, \qquad \sum_b \tilde{f}^b(\mathbf{x}) \tilde{f}^b(\mathbf{x})^* = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{1.45}$$

to re-expand

$$\Psi(\mathbf{x},t) = \sum_b \tilde{f}^b(\mathbf{x}) \tilde{\Psi}_b(t), \tag{1.46}$$

with

$$\tilde{\Psi}_b(t) = \int d^3x\, \tilde{f}^b(\mathbf{x})^*\, \Psi(\mathbf{x},t). \tag{1.47}$$

Inserting (1.156) shows that the components are related to each other by

$$\tilde{\Psi}_b(t) = \sum_a \left[\int d^3x\, \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}) \right] \Psi_a(t). \tag{1.48}$$

It is useful to write the scalar products between two basis functions in the so-called *bracket notation* as

$$\langle \tilde{b} | a \rangle \equiv \int d^3x\, \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}). \tag{1.49}$$

In this notation, the components of the state vector $\Psi(\mathbf{x},t)$ in (1.157), (1.160) are

$$\begin{aligned} \Psi_a(t) &= \langle a | \Psi(t) \rangle, \\ \tilde{\Psi}_b(t) &= \langle \tilde{b} | \Psi(t) \rangle. \end{aligned} \tag{1.50}$$

The transformation formula (1.161) takes the form

$$\langle \tilde{b} | \Psi(t) \rangle = \sum_a \langle \tilde{b} | a \rangle \langle a | \Psi(t) \rangle. \tag{1.51}$$

The right-hand side of this equation may be formally viewed as a result of inserting the abstract relation

$$\sum_a |a\rangle\langle a| = 1 \tag{1.52}$$

between $\langle\tilde{b}|$ and $|\Psi(t)\rangle$ on the left-hand side:

$$\langle\tilde{b}|\Psi(t)\rangle = \langle\tilde{b}|1|\Psi(t)\rangle = \sum_a \langle\tilde{b}|a\rangle\langle a|\Psi(t)\rangle. \tag{1.53}$$

Since this expansion is only possible if the functions $f^b(\mathbf{x})$ form a complete basis, the relation (1.165) is alternative, abstract way of stating the completeness of the basis functions. It is therefore equivalent to (1.155) and also referred to as a *completeness relation* à la Dirac.

Since the scalar product are written in the form of brackets $\langle a|a'\rangle$, Dirac called the formal objects $\langle a|$ and $|a'\rangle$, from which the brackets are composed, *bra* and *ket*, respectively. In the bracket notation, the orthonormality of the basis $f^a(\mathbf{x})$ and $g^b(\mathbf{x})$ may be expressed as follows:

$$\begin{aligned} \langle a|a'\rangle &= \int d^3x\, f^a(\mathbf{x})^* f^{a'}(\mathbf{x}) = \delta^{aa'}, \\ \langle\tilde{b}|\tilde{b}'\rangle &= \int d^3x\, \tilde{f}^b(\mathbf{x})^* \tilde{f}^{b'}(\mathbf{x}) = \delta^{bb'}. \end{aligned} \tag{1.54}$$

A special set of basis functions called *local basis functions* is of particular importance. It may be constructed in the following fashion: Imagine the continuum of space points to be coarse-grained into a cubic lattice of mesh size ϵ, at positions

$$\mathbf{x}^{\mathbf{n}} = (n_1, n_2, n_3)\epsilon, \qquad n_{1,2,3} = 0, \pm 1, \pm 2, \dots\ . \tag{1.55}$$

Let $h^{\mathbf{n}}(\mathbf{x})$ be a function that vanishes everywhere in space, except in a cube of size ϵ^3 centered around $\mathbf{x}^{\mathbf{n}}$, i.e., for each component x_i of $\mathbf{x}$,

$$h^{\mathbf{n}}(\mathbf{x}) = \begin{cases} 1/\sqrt{\epsilon^3} & |x_i - x_i^{\mathbf{n}}| \le \epsilon/2, \quad i = 1, 2, 3. \\ 0 & \text{otherwise.} \end{cases} \tag{1.56}$$

These functions are certainly orthonormal:

$$\int d^3x\, h^{\mathbf{n}}(\mathbf{x})^* h^{\mathbf{n}'}(\mathbf{x}) = \delta^{\mathbf{n}\mathbf{n}'}. \tag{1.57}$$

Consider now the expansion

$$\Psi(\mathbf{x}, t) = \sum_{\mathbf{n}} h^{\mathbf{n}}(\mathbf{x})\Psi_{\mathbf{n}}(t) \tag{1.58}$$

with the coefficients

$$\Psi_{\mathbf{n}}(t) = \int d^3x\, h^{\mathbf{n}}(\mathbf{x})^* \Psi(\mathbf{x}, t) \approx \sqrt{\epsilon^3}\,\Psi(\mathbf{x}^{\mathbf{n}}, t). \tag{1.59}$$

It provides an excellent approximation to the true wave function $\Psi(\mathbf{x},t)$, as long as the mesh size ϵ is much smaller than the scale over which $\Psi(\mathbf{x},t)$ varies. In fact, if $\Psi(\mathbf{x},t)$ is integrable, the integral over the sum (1.171) will always converge to $\Psi(\mathbf{x},t)$. The same convergence of discrete approximations is found in any scalar product, and thus in any observable probability amplitudes. They can all be calculated with arbitrary accuracy knowing the discrete components of the type (1.172) in the limit $\epsilon \longrightarrow 0$. The functions $h^{\mathbf{n}}(\mathbf{x})$ may therefore be used as an approximate basis in the same way as the previous basis functions $f^a(\mathbf{x}), g^b(\mathbf{x})$, with any desired accuracy depending on the choice of ϵ. It is convenient to introduce abstract bra and ket vectors associated with the basis functions $h^{\mathbf{n}}(\mathbf{x})$, denoting them by $\langle\mathbf{x}^{\mathbf{n}}|$ and $|\mathbf{x}^{\mathbf{n}}\rangle$, respectively, and writing the orthonormality relation (1.170) in bracket notation as

$$\langle\mathbf{x}^{\mathbf{n}}|\mathbf{x}^{\mathbf{n}'}\rangle \equiv \int d^3x\, h^{\mathbf{n}}(\mathbf{x})^* h^{\mathbf{n}'}(\mathbf{x}) = \delta^{\mathbf{n}\mathbf{n}'}. \tag{1.60}$$

The components $\Psi_{\mathbf{n}}(t)$ may be considered as the scalar products

$$\Psi_{\mathbf{n}}(t) \equiv \langle\mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle \approx \sqrt{\epsilon^3}\Psi(\mathbf{x}^{\mathbf{n}},t). \tag{1.61}$$

Changes of basis vectors, for instance from $|\mathbf{x}^{\mathbf{n}}\rangle$ to the states $|a\rangle$, can be performed according to the rules developed above by inserting an abstract completeness relation of the type (1.165). Thus we may expand

$$\Psi_{\mathbf{n}}(t) = \langle\mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle = \sum_a \langle\mathbf{x}^{\mathbf{n}}|a\rangle\langle a|\Psi(t)\rangle. \tag{1.62}$$

Also the inverse relation is true:

$$\langle a|\Psi(t)\rangle = \sum_{\mathbf{n}} \langle a|\mathbf{x}^{\mathbf{n}}\rangle\langle\mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle. \tag{1.63}$$

This is, of course, just an approximation to the integral

$$\int d^3x\, f^a(\mathbf{x})^* \langle\mathbf{x}|\Psi(t)\rangle. \tag{1.64}$$

The completeness of the basis $h^{\mathbf{n}}(\mathbf{x})$ may therefore be expressed via the abstract relation

$$\sum_{\mathbf{n}} |\mathbf{x}^{\mathbf{n}}\rangle\langle\mathbf{x}^{\mathbf{n}}| \approx 1. \tag{1.65}$$

The approximate sign turns into an equality sign in the limit of zero mesh size, $\epsilon \longrightarrow 0$.

In ordinary calculus, finer and finer sums are eventually replaced by integrals. The same thing is done here. We define new continuous scalar products

$$\langle\mathbf{x}|\Psi(t)\rangle \approx \frac{1}{\sqrt{\epsilon^3}}\langle\mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle, \tag{1.66}$$

where $\mathbf{x}^{\mathbf{n}}$ are the lattice points closest to $\mathbf{x}$. With (1.174), the right-hand side is equal to $\Psi(\mathbf{x}^{\mathbf{n}},t)$.

In the limit $\epsilon \longrightarrow 0$, $\mathbf{x}$ and $\mathbf{x}^{\mathbf{n}}$ coincide and we have

$$\langle \mathbf{x}|\Psi(t)\rangle \equiv \Psi(\mathbf{x},t). \tag{1.67}$$

The completeness relation can be used to write

$$\begin{aligned} \langle a|\Psi(t)\rangle &\approx \sum_{\mathbf{n}} \langle a|\mathbf{x}^{\mathbf{n}}\rangle\langle \mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle \\ &\approx \sum_{\mathbf{n}} \epsilon^3 \langle a|\mathbf{x}\rangle\langle \mathbf{x}|\Psi(t)\rangle\Big|_{\mathbf{x}=\mathbf{x}^{\mathbf{n}}} , \end{aligned} \tag{1.68}$$

which in the limit $\epsilon \longrightarrow 0$ becomes

$$\langle a|\Psi(t)\rangle = \int d^3x\, \langle a|\mathbf{x}\rangle\langle \mathbf{x}|\Psi(t)\rangle. \tag{1.69}$$

This may be viewed as the result of inserting the formal completeness relation of the limiting local bra and ket basis vectors $\langle \mathbf{x}|$ and $|\mathbf{x}\rangle$,

$$\int d^3x\, |\mathbf{x}\rangle\langle \mathbf{x}| = 1, \tag{1.70}$$

evaluated between the vectors $\langle a|$ and $|\Psi(t)\rangle$.

With the limiting local basis, the wave functions can be treated as components of the state vectors $|\Psi(t)\rangle$ with respect to the local basis $|\mathbf{x}\rangle$ in the same way as any other set of components in an arbitrary basis $|a\rangle$. In fact, the expansion

$$\langle a|\Psi(t)\rangle = \int d^3x\, \langle a|\mathbf{x}\rangle\langle \mathbf{x}|\Psi(t)\rangle \tag{1.71}$$

may be viewed as a re-expansion of a component of $|\Psi(t)\rangle$ in one basis, $|a\rangle$, into those of another basis, $|\mathbf{x}\rangle$, just as in (1.164).

In order to express all these transformation properties in a most compact notation, it has become customary to deal with an arbitrary physical state vector in a *basis-independent* way and denote it by a ket vector $|\Psi(t)\rangle$. This vector may be specified in any convenient basis by multiplying it with the corresponding completeness relation

$$\sum_a |a\rangle\langle a| = 1, \tag{1.72}$$

resulting in the expansion

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle. \tag{1.73}$$

This can be multiplied with any bra vector, say $\langle b|$, from the left to obtain the expansion formula (1.166):

$$\langle b|\Psi(t)\rangle = \sum_a \langle b|a\rangle\langle a|\Psi(t)\rangle. \tag{1.74}$$

In particular, the completeness relation of the local basis states

$$\int d^3x\,|\mathbf{x}\rangle\langle\mathbf{x}| = 1 \tag{1.75}$$

leads to the expansion

$$|\Psi(t)\rangle = \int d^3x\,|\mathbf{x}\rangle\langle\mathbf{x}|\Psi(t)\rangle, \tag{1.76}$$

in which the wave function $\Psi(\mathbf{x},t) = \langle\mathbf{x}|\Psi(t)\rangle$ plays the role of an $\mathbf{x}$th component of the state vector $|\Psi(t)\rangle$ in the local basis $|\mathbf{x}\rangle$. This, in turn, is the limit of the discrete basis vectors $|\mathbf{x}^{\mathbf{n}}\rangle$,

$$|\mathbf{x}\rangle \approx \frac{1}{\sqrt{\epsilon^3}}\,|\mathbf{x}^{\mathbf{n}}\rangle\,, \tag{1.77}$$

with $\mathbf{x}^{\mathbf{n}}$ being the lattice points closest to $\mathbf{x}$.

A vector can be described equally well in bra or in ket form. To apply the above formalism consistently, we observe that the scalar products

$$\begin{aligned}\langle a|\tilde{b}\rangle &= \int d^3x\, f^a(\mathbf{x})^*\tilde{f}^b(\mathbf{x}),\\ \langle\tilde{b}|a\rangle &= \int d^3x\, \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x})\end{aligned} \tag{1.78}$$

satisfy the identity

$$\langle\tilde{b}|a\rangle \equiv \langle a|\tilde{b}\rangle^*. \tag{1.79}$$

Therefore, when expanding a ket vector as

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle, \tag{1.80}$$

or a bra vector as

$$\langle\Psi(t)| = \sum_a \langle\Psi(t)|a\rangle\langle a|, \tag{1.81}$$

a multiplication of the first equation with the bra $\langle\mathbf{x}|$ and of the second with the ket $|\mathbf{x}\rangle$ produces equations which are complex-conjugate to each other.

Dirac's bra-ket formalism is elegant and easy to handle. As far as the vectors $|\mathbf{x}\rangle$ are concerned there is, however, one inconsistency with some fundamental postulates of quantum mechanics: When introducing state vectors, the norm was required to be unity in order to permit a proper probability interpretation of single-particle states. The limiting states $|\mathbf{x}\rangle$ introduced above do not satisfy this requirement. In fact, the scalar product between two different states $\langle\mathbf{x}|$ and $|\mathbf{x}'\rangle$ is

$$\langle\mathbf{x}|\mathbf{x}'\rangle \approx \frac{1}{\epsilon^3}\langle\mathbf{x}^{\mathbf{n}}|\mathbf{x}^{\mathbf{n}'}\rangle = \frac{1}{\epsilon^3}\delta^{\mathbf{n}\mathbf{n}'}, \tag{1.82}$$

where $\mathbf{x}^{\mathbf{n}}$ and $\mathbf{x}^{\mathbf{n}'}$ are the lattice points closest to $\mathbf{x}$ and $\mathbf{x}'$. For $\mathbf{x} \neq \mathbf{x}'$, the states are orthogonal. For $\mathbf{x} = \mathbf{x}'$, on the other hand, the limit $\epsilon \to 0$ is infinite, approached in such a way that

$$\epsilon^3\sum_{\mathbf{n}'}\frac{1}{\epsilon^3}\delta^{\mathbf{n}\mathbf{n}'} = 1. \tag{1.83}$$

Therefore, the limiting state $|\mathbf{x}\rangle$ is not a properly normalizable vector in the Hilbert space. For the sake of elegance, it is useful to weaken the requirement of normalizability (1.24) by admitting the limiting states $|\mathbf{x}\rangle$ to the physical Hilbert space. In fact, one admits all states which can be obtained by a limiting sequence from properly normalized state vectors.

The scalar product between states $\langle\mathbf{x}|\mathbf{x}'\rangle$ is not a proper function. One denotes this scalar product by the symbol $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ and writes

$$\langle\mathbf{x}|\mathbf{x}'\rangle \equiv \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{1.84}$$

where $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ is defined by its approximant for $\epsilon \to 0$:

$$\delta^{(3)}(\mathbf{x}-\mathbf{x}') \approx \frac{1}{\epsilon^3}\delta^{\,\mathbf{n}\mathbf{n}'}. \tag{1.85}$$

The right-hand side vanishes everywhere except in the infinitely narrow ϵ-neighborhood of $\mathbf{x} \approx \mathbf{x}'$. Thus, in the limit $\epsilon \to 0$, the symbol $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ satisfies

$$\delta^{(3)}(\mathbf{x}-\mathbf{x}') = 0 \quad \text{for} \quad \mathbf{x} \neq \mathbf{x}'. \tag{1.86}$$

At $\mathbf{x}=\mathbf{x}'$, $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ is so large that its volume integral is unity:

$$\int d^3x'\,\delta^{(3)}(\mathbf{x}-\mathbf{x}') = 1. \tag{1.87}$$

Obviously, there exists no proper function that can satisfy both requirements, (1.86) and (1.87). Only the approximants to the δ-function are proper functions. In this respect, the scalar product $\langle\mathbf{x}|\mathbf{x}'\rangle$ behaves just like the states $|\mathbf{x}\rangle$ themselves: Both are $\epsilon \to 0$ -limits of properly defined mathematical objects.

Once we admit the generalized states $|\mathbf{x}\rangle$ to the Hilbert space, we should also admit the scalar products $\langle\mathbf{x}|\mathbf{x}'\rangle$ to the space of wave functions. They are called *generalized functions* or *distributions*. Mathematically, a distribution such as $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ is defined by its effect, under a spatial integral, on a certain class of functions called *test functions* $f(\mathbf{x})$. These are arbitrarily often differentiable functions with a sufficiently fast falloff at spatial infinity. Let $f(\mathbf{x})$ be such a test function; then $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ is defined by the relation, valid for any $f(\mathbf{x})$:

$$\int d^3x\,\delta^{(3)}(\mathbf{x}-\mathbf{x}')f(\mathbf{x}') = f(\mathbf{x}). \tag{1.88}$$

In quantum mechanics, the role of the test functions is played by the wave packets $\Psi(\mathbf{x},t)$. Like the bra-ket formalism, the generalized function $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ was introduced by Dirac, and for this reason it is called the *Dirac δ-function.*

In terms of the bra-ket notation, the Schrödinger equation can be expressed in a basis-independent way as an operator equation

$$\hat{H}|\Psi(t)\rangle \equiv H(\hat{\mathbf{p}},\hat{\mathbf{x}},t)|\Psi(t)\rangle = i\hbar\partial_t|\Psi(t)\rangle, \tag{1.89}$$

to be supplemented by the following specifications of the canonical operators:

$$\begin{aligned} \langle \mathbf{x}|\hat{\mathbf{p}} &\equiv -i\hbar\partial_{\mathbf{x}}\langle \mathbf{x}|, & (1.90)\\ \langle \mathbf{x}|\hat{\mathbf{x}} &\equiv \mathbf{x}\langle \mathbf{x}|. & (1.91) \end{aligned}$$

Any matrix element can be obtained from these equations by multiplication from the right with an arbitrary ket vector; for instance with the local basis vector $|\mathbf{x}'\rangle$:

$$\begin{aligned} \langle \mathbf{x}|\hat{\mathbf{p}}|\mathbf{x}'\rangle &= -i\hbar\partial_{\mathbf{x}}\langle \mathbf{x}|\mathbf{x}'\rangle = -i\hbar\partial_{\mathbf{x}}\delta^{(3)}(\mathbf{x}-\mathbf{x}'), & (1.92)\\ \langle \mathbf{x}|\hat{\mathbf{x}}|\mathbf{x}'\rangle &= \mathbf{x}\langle \mathbf{x}|\mathbf{x}'\rangle = \mathbf{x}\delta^{(3)}(\mathbf{x}-\mathbf{x}'). & (1.93) \end{aligned}$$

The original differential form of the Schrödinger equation (1.17) follows by multiplying the basis-independent Schrödinger equation (1.89) with the bra vector $\langle \mathbf{x}|$ from the left:

$$\begin{aligned} \langle \mathbf{x}|H(\hat{\mathbf{p}},\hat{\mathbf{x}},t)|\Psi(t)\rangle &= H(-i\hbar\partial_{\mathbf{x}},\mathbf{x},t)\langle \mathbf{x}|\Psi(t)\rangle \\ &= i\hbar\partial_t\langle \mathbf{x}|\Psi(t)\rangle. \end{aligned} \qquad (1.94)$$

Obviously, $\hat{\mathbf{p}}$ and $\hat{\mathbf{x}}$ are Hermitian matrices in any basis,

$$\begin{aligned} \langle a|\hat{\mathbf{p}}|a'\rangle &= \langle a'|\hat{\mathbf{p}}|a\rangle^*, & (1.95)\\ \langle a|\hat{\mathbf{x}}|a'\rangle &= \langle a'|\hat{\mathbf{x}}|a\rangle^*, & (1.96) \end{aligned}$$

and so is the Hamiltonian

$$\langle a|\hat{H}|a'\rangle = \langle a'|\hat{H}|a\rangle^*, \qquad (1.97)$$

as long as it has the form (1.28).

The most general basis-independent operator that can be constructed in the generalized Hilbert space spanned by the states $|\mathbf{x}\rangle$ is some function of $\hat{\mathbf{p}},\hat{\mathbf{x}},t$,

$$\hat{O}(t) \equiv O(\hat{\mathbf{p}},\hat{\mathbf{x}},t). \qquad (1.98)$$

In general, such an operator is called Hermitian if all its matrix elements have this property. The Hermitian-adjoint operator $O^\dagger(t)$ is defined by the matrix elements

$$\langle a|O^\dagger(t)|a'\rangle \equiv \langle a'|O(t)|a\rangle^*. \qquad (1.99)$$

With this definition, we can rephrase the equations (1.95) - (1.97) in the basis-independent form

$$\begin{aligned} \hat{\mathbf{p}} &= \hat{\mathbf{p}}^\dagger, \\ \hat{\mathbf{x}} &= \hat{\mathbf{x}}^\dagger, \\ \hat{H} &= \hat{H}^\dagger. \end{aligned} \qquad (1.100)$$

1.3 Observables

Changes of basis vectors are an important tool in analyzing the physically observable content of a wave vector. Let $A = A(\mathbf{p}, \mathbf{x})$ be an arbitrary time-independent real function of the phase space variables $\mathbf{p}$ and $\mathbf{x}$. Important examples for such an A are $\mathbf{p}$ and $\mathbf{x}$ themselves, the Hamiltonian $H(\mathbf{p}, \mathbf{x})$, and the angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$. Quantum-mechanically, there will be an observable operator associated with each such quantity. It is obtained by simply replacing the variables $\mathbf{p}$ and $\mathbf{x}$ in A by the corresponding operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{x}}$:

$$\hat{A} \equiv A(\hat{\mathbf{p}}, \hat{\mathbf{x}}). \tag{1.101}$$

This replacement rule is the extension of the correspondence principle for the Hamilton operator (1.18) to more general functions in phase space, converting them into observable operators. It must be assumed that the replacement leads to a unique Hermitian operator, i.e., that there is no ordering problem of the type discussed in context with the Hamiltonian (1.28).[5] If there are ambiguities, the naive correspondence principle is insufficient to determine the operators. A nonholonomic mapping procedure known as *quantum equivalence principle* will do the job, and seems to be in agreement with present-day axperimental data.[6]

Once an observable operator $\hat{A}$ is Hermitian, it has the useful property that the set of all eigenvectors $|a\rangle$ obtained by solving the equation

$$\hat{A}|a\rangle = a|a\rangle \tag{1.102}$$

can be used as a basis to span the Hilbert space. Among the eigenvectors, there is always a choice of orthonormal vectors $|a\rangle$ fulfilling the completeness relation

$$\sum_a |a\rangle\langle a| = 1. \tag{1.103}$$

The vectors $|a\rangle$ can be used to extract physical information concerning the observable A from arbitrary state vector $|\Psi(t)\rangle$. For this we expand this vector in the basis $|a\rangle$:

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle. \tag{1.104}$$

The components

$$\langle a|\Psi(t)\rangle \tag{1.105}$$

yield the probability amplitude for measuring the eigenvalue a for the observable quantity A.

The wave function $\Psi(\mathbf{x}, t)$ itself is an example of this interpretation. If we write it as

$$\Psi(\mathbf{x}, t) = \langle \mathbf{x}|\Psi(t)\rangle, \tag{1.106}$$

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[5] Note that this is true for the angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$.

[6] For a detailed discussion of this topic see Sections 1.5–1.7 and Chapters 10–11 in H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, World Scientific, Singapore, 1995.

it gives the probability amplitude for measuring the eigenvalues $\mathbf{x}$ of the position operator $\hat{\mathbf{x}}$, i.e., $|\Psi(\mathbf{x},t)|^2$ is the probability density in $\mathbf{x}$-space.

Let us now look at the momentum $\hat{\mathbf{p}}$. Its eigenstates are given by the eigenvalue equation

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle. \tag{1.107}$$

By multiplying this with $\langle\mathbf{x}|$ from the left and using (1.90), we find the differential equation

$$\langle\mathbf{x}|\hat{\mathbf{p}}|\mathbf{p}\rangle = -i\hbar\partial_{\mathbf{x}}\langle\mathbf{x}|\mathbf{p}\rangle = \mathbf{p}\langle\mathbf{x}|\mathbf{p}\rangle. \tag{1.108}$$

The solution is

$$\langle\mathbf{x}|\mathbf{p}\rangle \propto e^{i\mathbf{p}\mathbf{x}/\hbar}. \tag{1.109}$$

Up to a normalization factor, this is just a plane wave introduced before in Eq. (1.1) to describe free particles of momentum $\mathbf{p}$.

In order for the states $|\mathbf{p}\rangle$ to have a finite norm, the system must be confined to a finite volume, say a cubic box of length L and volume L^3. Assuming periodic boundary conditions, the momenta are discrete with values

$$\mathbf{p}^{\mathbf{m}} = \frac{2\pi\hbar}{L}(m_1, m_2, m_3), \quad m_i = 0, \pm 1, \pm 2, \dots \ . \tag{1.110}$$

Then we adjust the factor in front of $\exp(i\mathbf{p}^{\mathbf{m}}\mathbf{x}/\hbar)$ to achieve unit normalization

$$\langle\mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle = \frac{1}{\sqrt{L^3}}\exp\left(i\mathbf{p}^{\mathbf{m}}\mathbf{x}/\hbar\right), \tag{1.111}$$

and the discrete states $|\mathbf{p}^{\mathbf{m}}\rangle$ satisfy

$$\int d^3x \, |\langle\mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle|^2 = 1. \tag{1.112}$$

The states $|\mathbf{p}^{\mathbf{m}}\rangle$ are complete:

$$\sum_{\mathbf{m}} |\mathbf{p}^{\mathbf{m}}\rangle\langle\mathbf{p}^{\mathbf{m}}| = 1. \tag{1.113}$$

We may use this relation and the matrix elements $\langle\mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle$ to expand any wave function within the box as

$$\Psi(\mathbf{x},t) = \langle\mathbf{x}|\Psi(t)\rangle = \sum_{\mathbf{m}}\langle\mathbf{x}|\mathbf{p}^{\mathbf{m}}\rangle\langle\mathbf{p}^{\mathbf{m}}|\Psi(t)\rangle. \tag{1.114}$$

If the box is very large, $L \to \infty$, the sum over the discrete momenta $\mathbf{p}^{\mathbf{m}}$ can be approximated by an integral over phase space,[7]

$$\sum_{\mathbf{m}} \approx \int\int \frac{d^3p\, d^3x}{(2\pi\hbar)^3} = \int \frac{d^3p\, V}{(2\pi\hbar)^3}. \tag{1.115}$$

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[7] An exception occurs in the theory of superfluid helium where the single state $\mathbf{p} = 0$ requires a separate treatment since it accumulates a large number of particles in what is called a *Bose-Einstein condensate*. See L.D. Landau and E.M. Lifshitz, *Statistical Mechanics*, Pergamon Press, London, 1958, p. 169.

For large L, the states $\mathbf{p}^{\mathbf{m}}$ may be used to define basis vectors

$$|\mathbf{p}\rangle \approx \sqrt{V}|\mathbf{p}^{\mathbf{m}}\rangle, \tag{1.116}$$

in the same way as $|\mathbf{x}^{\mathbf{n}}\rangle$ was previously used to define $|\mathbf{x}\rangle \sim (1/\sqrt{\epsilon^3})|\mathbf{x}^{\mathbf{n}}\rangle$ [recall Eq. (1.190)]. The limiting continuous momentum states $|\mathbf{p}\rangle$ are orthogonal,

$$\langle\mathbf{p}|\mathbf{p}'\rangle = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{p}'), \tag{1.117}$$

with $\delta^{(3)}(\mathbf{p}-\mathbf{p}')$ being again the Dirac δ-function. These states satisfy the completeness relation

$$\int\frac{d^3p}{(2\pi\hbar)^3}|\mathbf{p}\rangle\langle\mathbf{p}| = 1. \tag{1.118}$$

In the limit $L\to\infty$, the expansion (1.114) becomes then

$$\psi(\mathbf{x},t) = \int\frac{d^3p}{(2\pi\hbar)^3}\langle\mathbf{x}|\mathbf{p}\rangle\langle\mathbf{p}|\psi(t)\rangle, \tag{1.119}$$

with the continuous momentum eigenfunctions

$$\langle\mathbf{x}|\mathbf{p}\rangle = \psi_{\mathbf{p}}(\mathbf{x}) = e^{i\mathbf{px}/\hbar}. \tag{1.120}$$

This coincides precisely with the Fourier decomposition introduced above in the description of a general particle wave $\psi(\mathbf{x},t)$ in (1.8), (1.9), with the identification

$$\langle\mathbf{p}|\psi(t)\rangle = f(\mathbf{p})e^{-iE_{\mathbf{p}}t/\hbar}. \tag{1.121}$$

The fequent apparence of factors $2\pi\hbar$ with δ-functions and integration measures in momentum space makes it convenient to define the modified δ-functions and integration measures

$$\bar{\delta}^{(D)}(\mathbf{p}) \equiv (2\pi\hbar)^D\delta^{(D)}(\mathbf{p}), \qquad \bar{d}^Dp \equiv \frac{d^Dp}{(2\pi\hbar)^D}, \tag{1.122}$$

the latter in analogy with $\hbar \equiv h/2\pi$. Then we may write orthogonality and completeness relations (1.117) and (1.118).

The bra-ket formalism accommodates naturally the technique of Fourier transforms. The Fourier inversion formula is found by simply inserting into $\langle\mathbf{p}|\Psi(t)\rangle$ a completeness relation $\int d^3x|\mathbf{x}\rangle\langle\mathbf{x}| = 1$ which yields

$$\begin{aligned}\langle\mathbf{p}|\Psi(t)\rangle &= \int d^3x\,\langle\mathbf{p}|\mathbf{x}\rangle\langle\mathbf{x}|\Psi(t)\rangle \\ &= \int d^3x\,e^{-i\mathbf{px}/\hbar}\Psi(\mathbf{x},t).\end{aligned} \tag{1.123}$$

The amplitudes $\langle\mathbf{p}|\Psi(t)\rangle$ are referred to as *momentum space wave functions.*

By inserting the completeness relation $\int d^3x|\mathbf{x}\rangle\langle\mathbf{x}| = 1$ between the momentum states on the left-hand side of the orthogonality relation (1.117, we obtain the Fourier representation of the δ-function

$$\begin{aligned} \langle\mathbf{p}|\mathbf{p}'\rangle &= \int d^3x\, \langle\mathbf{p}|\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{p}'\rangle \\ &= \int d^3x\, e^{-i(\mathbf{p}-\mathbf{p}')\mathbf{x}/\hbar}. \end{aligned} \tag{1.124}$$

We have seen before [see the discussion after (1.8), (1.9)] that the amplitudes in real space and those in momentum space have widths inversely proportional to each other, due to the properties of Fourier analysis. If a wave packet is localized in real space with a width $\Delta\mathbf{x}$, its momentum space wave function has a width $\Delta\mathbf{p}$ given by

$$\Delta\mathbf{x}\,\Delta\mathbf{p} \sim \hbar. \tag{1.125}$$

From the Hilbert space point of view this uncertainty relation can be shown to be a consequence of the fact that the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$ do not commute with each other, but the components satisfy the canonical commutation rules

$$\begin{aligned} [\hat{p}_i, \hat{x}_j] &= -i\hbar\delta_{ij}, \\ [\hat{x}_i, \hat{x}_j] &= 0, \\ [\hat{p}_i, \hat{p}_j] &= 0. \end{aligned} \tag{1.126}$$

In general, if an observable operator $\hat{A}$ is measured sharply to have the value a in one state, this state must be an eigenstate of $\hat{A}$ with an eigenvalue a:

$$\hat{A}|a\rangle = a|a\rangle. \tag{1.127}$$

This follows from the expansion

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle, \tag{1.128}$$

in which $|\langle a|\Psi(t)\rangle|^2$ is the probability to measure an arbitrary eigenvalue a. If this probability is sharply focussed at a specific value of a, the state necessarily coincides with $|a\rangle$.

Given the set of all eigenstates $|a\rangle$ of $\hat{A}$, we may ask under what circumstances another observable, say $\hat{B}$, can be measured sharply in each of these states. The requirement implies that the states $|a\rangle$ are also eigenstates of $\hat{B}$,

$$\hat{B}|a\rangle = b_a|a\rangle, \tag{1.129}$$

with some a-dependent eigenvalue b_a. If this is true for all $|a\rangle$,

$$\hat{B}\hat{A}|a\rangle = b_a a|a\rangle = a b_a|a\rangle = \hat{A}\hat{B}|a\rangle, \tag{1.130}$$

the operators $\hat{A}$ and $\hat{B}$ necessarily commute:

$$[\hat{A}, \hat{B}] = 0. \tag{1.131}$$

Conversely, it can be shown that a vanishing commutator is also sufficient for two observable operators to be simultaneously diagonalizable and thus to allow for simultaneous sharp measurements.

All this development can be extended to systems of N distinguishable mass points with Cartesian coordinates freedom $\mathbf{x}_1, \ldots, \mathbf{x}_N$. If $H(\mathbf{p}_\nu, \mathbf{x}_\nu, t)$ is the Hamiltonian, the Schrödinger equation becomes

$$H(\hat{\mathbf{p}}_\nu, \hat{\mathbf{x}}_\nu, t)|\Psi(t)\rangle = i\hbar\partial_t|\Psi(t)\rangle. \tag{1.132}$$

We may introduce a complete local basis $|\mathbf{x}_1, \ldots, \mathbf{x}_N\rangle$ with the properties

$$\begin{aligned} &\langle \mathbf{x}_1, \ldots, \mathbf{x}_N|\mathbf{x}'_1, \ldots, \mathbf{x}'_N\rangle = \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \cdots \delta^{(3)}(\mathbf{x}_N - \mathbf{x}'_N), \\ &\int d^3x_1 \cdots d^3x_N |\mathbf{x}_1, \ldots, \mathbf{x}_N\rangle\langle \mathbf{x}_1, \ldots, \mathbf{x}_N| = 1, \end{aligned} \tag{1.133}$$

and define

$$\begin{aligned} \langle \mathbf{x}_1, \ldots, \mathbf{x}_N|\hat{\mathbf{p}}_\nu &= -i\hbar\partial_{\mathbf{x}_\nu}\langle \mathbf{x}_1, \ldots, \mathbf{x}_N|, \\ \langle \mathbf{x}_1, \ldots, \mathbf{x}_N|\hat{\mathbf{x}}_\nu &= \mathbf{x}_\nu\langle \mathbf{x}_1, \ldots, \mathbf{x}_N|. \end{aligned} \tag{1.134}$$

The Schrödinger equation for N particles (1.34) follows from (1.132) by multiplying it from the left with the bra vectors $\langle \mathbf{x}_1, \ldots, \mathbf{x}_N|$. In the same way, all other formulas given above can be generalized to N-body state vectors.

1.4 Time Evolution Operator

If the Hamilton operator has the special form $\hat{H} = H(\hat{\mathbf{p}}, \hat{\mathbf{x}})$, i.e., if it contains no explicit time dependence, the basis-independent Schrödinger equation (1.89) can be integrated to find the wave function $|\Psi(t)\rangle$ at any time t_b from the state at any other time t_a

$$|\Psi(t_b)\rangle = e^{-i(t_b-t_a)\hat{H}/\hbar}|\Psi(t_a)\rangle. \tag{1.135}$$

The operator

$$\hat{U}(t_b, t_a) = e^{-i(t_b-t_a)\hat{H}/\hbar} \tag{1.136}$$

is called the *time evolution operator*. Its inverse is obtained by interchanging the order of t_b and t_a:

$$\hat{U}^{-1}(t_b, t_a) \equiv e^{i(t_b-t_a)\hat{H}/\hbar} = \hat{U}(t_a, t_b). \tag{1.137}$$

As an exponential of i times a Hermitian operator, $\hat{U}$ is a *unitary operator* satisfying

$$\hat{U}^\dagger = \hat{U}^{-1}. \tag{1.138}$$

Indeed,

$$\begin{aligned}\hat{U}^\dagger(t_b,t_a) &= e^{i(t_b-t_a)\hat{H}^\dagger/\hbar}\\ &= e^{i(t_b-t_a)\hat{H}/\hbar} = \hat{U}^{-1}(t_b,t_a).\end{aligned} \tag{1.139}$$

If $H(\hat{\mathbf{p}},\hat{\mathbf{x}},t)$ depends explicitly on time, the integration of the Schrödinger equation (1.89) is somewhat more involved. The solution may be found iteratively: For $t_b > t_a$, the time interval is sliced into a large number $N+1$ of small pieces of thickness ϵ with $\epsilon \equiv (t_b-t_a)/(N+1)$, slicing once at each time $t_n = t_a + n\epsilon$ for $n = 0,\dots,N+1$. We then use the Schrödinger equation (1.89) to relate the wave function in each slice approximately to the previous one:

$$\begin{aligned}|\Psi(t_a+\epsilon)\rangle &\approx \left(1-\frac{i}{\hbar}\int_{t_a}^{t_a+\epsilon} dt\,\hat{H}(t)\right)|\Psi(t_a)\rangle,\\ |\Psi(t_a+2\epsilon)\rangle &\approx \left(1-\frac{i}{\hbar}\int_{t_a+\epsilon}^{t_a+2\epsilon} dt\,\hat{H}(t)\right)|\Psi(t_a+\epsilon)\rangle,\\ &\vdots\\ |\Psi(t_a+(N+1)\epsilon)\rangle &\approx \left(1-\frac{i}{\hbar}\int_{t_a+N\epsilon}^{t_a+(N+1)\epsilon} dt\,\hat{H}(t)\right)|\Psi(t_a+N\epsilon)\rangle.\end{aligned} \tag{1.140}$$

The combination of these equations yields

$$\begin{aligned}|\Psi(t_b)\rangle &= \left(1-\frac{i}{\hbar}\int_{t_N}^{t_b} dt'_{N+1}\,\hat{H}(t'_{N+1})\right)\\ &\quad\times\left(1-\frac{i}{\hbar}\int_{t_{N-1}}^{t_N} dt'_N\,\hat{H}(t'_N)\right)\\ &\quad\times\cdots\times\left(1-\frac{i}{\hbar}\int_{t_a}^{t_1} dt'_1\,\hat{H}(t'_1)\right)|\Psi(t_a)\rangle.\end{aligned} \tag{1.141}$$

Thus the time displacement operator is given approximately by the product

$$\hat{U}(t_b,t_a) \approx \left(1-\frac{i}{\hbar}\int_{t_N}^{t_b} dt'_{N+1}\,\hat{H}(t'_{N+1})\right)\times\cdots\times\left(1-\frac{i}{\hbar}\int_{t_a}^{t_1} dt'_1\,\hat{H}(t'_1)\right). \tag{1.142}$$

By multiplying out the product and going to the limit $N\to\infty$ we find the series

$$\begin{aligned}\hat{U}(t_b,t_a) &= 1-\frac{i}{\hbar}\int_{t_a}^{t_b} dt_1\,\hat{H}(t_1) + \left(\frac{-i}{\hbar}\right)^2\int_{t_a}^{t_b} dt_2\int_{t_a}^{t_2} dt_1\,\hat{H}(t_2)\hat{H}(t_1)\\ &\quad+\left(\frac{-i}{\hbar}\right)^3\int_{t_a}^{t_b} dt_3\int_{t_a}^{t_3} dt_2\int_{t_a}^{t_2} dt_1\,\hat{H}(t_3)\hat{H}(t_2)\hat{H}(t_1)+\dots\,,\end{aligned} \tag{1.143}$$

known as the *Neumann-Liouville expansion* or *Dyson series*.

Note that each integral has the time arguments in the Hamilton operators ordered *causally*: Operators with later times stand to left of those with earlier times. It is useful to introduce a *time-ordering operator* which, when applied to an arbitrary product of operators,

$$\hat{O}_n(t_n)\cdots\hat{O}_1(t_1), \tag{1.144}$$

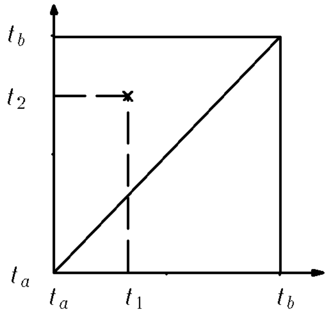

FIGURE 1.2 Illustration of the time-ordering procedure in Eq. (1.147).

reorders the times successively. More explicitly we define

$$\hat{T}(\hat{O}_n(t_n)\cdots\hat{O}_1(t_1)) \equiv \hat{O}_{i_n}(t_{i_n})\cdots\hat{O}_{i_1}(t_{i_1}), \tag{1.145}$$

where $t_{i_n},\dots,t_{i_1}$ are the times $t_n,\dots,t_1$ relabeled in the causal order, so that

$$t_{i_n} > t_{i_{n-1}} > \dots > t_{i_1}. \tag{1.146}$$

Any c-number factors in (1.145) can be pulled out in front of the $\hat{T}$ operator. With this formal operator, the Neumann-Liouville expansion can be rewritten in a more compact way. Take, for instance, the third term in (1.143)

$$\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1\, \hat{H}(t_2)\hat{H}(t_1). \tag{1.147}$$

The integration covers the triangle above the diagonal in the square $t_1, t_2 \in [t_a, t_b]$ in the (t_1, t_2) plane (see Fig. 1.2). By comparing this with the missing integral over the lower triangle

$$\int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1\, \hat{H}(t_2)\hat{H}(t_1) \tag{1.148}$$

we see that the two expressions coincide except for the order of the operators. This can be corrected with the use of a time-ordering operator $\hat{T}$. The expression

$$\hat{T}\int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1\, \hat{H}(t_2)\hat{H}(t_1) \tag{1.149}$$

is equal to (1.147) since it may be rewritten as

$$\int_{t_a}^{t_b} dt_2 \int_{t_2}^{t_b} dt_1\, \hat{H}(t_1)\hat{H}(t_2) \tag{1.150}$$

or, after interchanging the order of integration, as

$$\int_{t_a}^{t_b} dt_1 \int_{t_a}^{t_1} dt_2\, \hat{H}(t_1)\hat{H}(t_2). \tag{1.151}$$

Apart from the dummy integration variables $t_2 \leftrightarrow t_1$, this double integral coincides with (1.147). Since the time arguments are properly ordered, (1.147) can trivially be multiplied with the time-ordering operator. The conclusion of this discussion is that (1.147) can alternatively be written as

$$\frac{1}{2}\hat{T}\int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1\, \hat{H}(t_2)\hat{H}(t_1). \tag{1.152}$$

On the right-hand side, the integrations now run over the full square in the t_1, t_2-plane so that the two integrals can be factorized into

$$\frac{1}{2}\hat{T}\left(\int_{t_a}^{t_b} dt\, \hat{H}(t)\right)^2 . \tag{1.153}$$

Similarly, there are many possible orthonormal basis functions $f^a(\mathbf{x})$ in the Hilbert space which satisfy the orthogonality relation

$$\int d^3x\, f^a(\mathbf{x})^* f^{a'}(\mathbf{x}) = \delta^{aa'}, \tag{1.154}$$

and the completeness relation [which is here not automatically implied by (1.154)]

$$\sum_a f^a(\mathbf{x}) f^a(\mathbf{x})^* = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{1.155}$$

thus serving to expand

$$\Psi(\mathbf{x},t) = \sum_a f^a(\mathbf{x})\Psi_a(t), \tag{1.156}$$

with the coefficients

$$\Psi_a(t) = \int d^3x\, f^a(\mathbf{x})^*\, \Psi(\mathbf{x},t). \tag{1.157}$$

Certainly, one may use any other orthonormal basis $\tilde{f}^b(\mathbf{x})$ with the orthogonality and completeness relations

$$\int d^3x\, \tilde{f}^b(\mathbf{x})^* \tilde{f}^{b'}(\mathbf{x}) = \delta^{bb'}, \qquad \sum_b \tilde{f}^b(\mathbf{x})\tilde{f}^b(\mathbf{x})^* = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{1.158}$$

to re-expand

$$\Psi(\mathbf{x},t) = \sum_b \tilde{f}^b(\mathbf{x})\tilde{\Psi}_b(t), \tag{1.159}$$

with

$$\tilde{\Psi}_b(t) = \int d^3x\, \tilde{f}^b(\mathbf{x})^*\, \Psi(\mathbf{x},t). \tag{1.160}$$

Inserting (1.156) shows that the components are related to each other by

$$\tilde{\Psi}_b(t) = \sum_a \left[\int d^3x\, \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x})\right] \Psi_a(t). \tag{1.161}$$

It is useful to write the scalar products between two basis functions in the so-called *bracket notation* as

$$\langle\tilde{b}|a\rangle \equiv \int d^3x\, \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}). \tag{1.162}$$

In this notation, the components of the state vector $\Psi(\mathbf{x},t)$ in (1.157), (1.160) are

$$\begin{aligned} \Psi_a(t) &= \langle a|\Psi(t)\rangle, \\ \tilde{\Psi}_b(t) &= \langle\tilde{b}|\Psi(t)\rangle. \end{aligned} \tag{1.163}$$

The transformation formula (1.161) takes the form

$$\langle\tilde{b}|\Psi(t)\rangle = \sum_a \langle\tilde{b}|a\rangle\langle a|\Psi(t)\rangle. \tag{1.164}$$

The right-hand side of this equation may be formally viewed as a result of inserting the abstract relation

$$\sum_a |a\rangle\langle a| = 1 \tag{1.165}$$

between $\langle\tilde{b}|$ and $|\Psi(t)\rangle$ on the left-hand side:

$$\langle\tilde{b}|\Psi(t)\rangle = \langle\tilde{b}|1|\Psi(t)\rangle = \sum_a \langle\tilde{b}|a\rangle\langle a|\Psi(t)\rangle. \tag{1.166}$$

Since this expansion is only possible if the functions $f^b(\mathbf{x})$ form a complete basis, the relation (1.165) is alternative, abstract way of stating the completeness of the basis functions. It is therefore equivalent to (1.155) and also referred to as a *completeness relation* à la Dirac.

Since the scalar product are written in the form of brackets $\langle a|a'\rangle$, Dirac called the formal objects $\langle a|$ and $|a'\rangle$, from which the brackets are composed, *bra* and *ket*, respectively. In the bracket notation, the orthonormality of the basis $f^a(\mathbf{x})$ and $g^b(\mathbf{x})$ may be expressed as follows:

$$\begin{aligned} \langle a|a'\rangle &= \int d^3x\, f^a(\mathbf{x})^* f^{a'}(\mathbf{x}) = \delta^{aa'}, \\ \langle\tilde{b}|\tilde{b}'\rangle &= \int d^3x\, \tilde{f}^b(\mathbf{x})^* \tilde{f}^{b'}(\mathbf{x}) = \delta^{bb'}. \end{aligned} \tag{1.167}$$

A special set of basis functions called *local basis functions* is of particular importance. It may be constructed in the following fashion: Imagine the continuum of space points to be coarse-grained into a cubic lattice of mesh size ϵ, at positions

$$\mathbf{x}^{\mathbf{n}} = (n_1, n_2, n_3)\epsilon, \qquad n_{1,2,3} = 0, \pm 1, \pm 2, \dots\ . \tag{1.168}$$

Let $h^{\mathbf{n}}(\mathbf{x})$ be a function that vanishes everywhere in space, except in a cube of size ϵ^3 centered around $\mathbf{x}^{\mathbf{n}}$, i.e., for each component x_i of $\mathbf{x}$,

$$h^{\mathbf{n}}(\mathbf{x}) = \begin{cases} 1/\sqrt{\epsilon^3} & |x_i - x_i^{\mathbf{n}}| \leq \epsilon/2, \quad i = 1,2,3. \\ 0 & \text{otherwise.} \end{cases} \tag{1.169}$$

These functions are certainly orthonormal:

$$\int d^3x \, h^{\mathbf{n}}(\mathbf{x})^* h^{\mathbf{n}'}(\mathbf{x}) = \delta^{\mathbf{n}\mathbf{n}'}. \tag{1.170}$$

Consider now the expansion

$$\Psi(\mathbf{x},t) = \sum_{\mathbf{n}} h^{\mathbf{n}}(\mathbf{x})\Psi_{\mathbf{n}}(t) \tag{1.171}$$

with the coefficients

$$\Psi_{\mathbf{n}}(t) = \int d^3x \, h^{\mathbf{n}}(\mathbf{x})^* \Psi(\mathbf{x},t) \approx \sqrt{\epsilon^3}\Psi(\mathbf{x}^{\mathbf{n}},t). \tag{1.172}$$

It provides an excellent approximation to the true wave function $\Psi(\mathbf{x},t)$, as long as the mesh size ϵ is much smaller than the scale over which $\Psi(\mathbf{x},t)$ varies. In fact, if $\Psi(\mathbf{x},t)$ is integrable, the integral over the sum (1.171) will always converge to $\Psi(\mathbf{x},t)$. The same convergence of discrete approximations is found in any scalar product, and thus in any observable probability amplitudes. They can all be calculated with arbitrary accuracy knowing the discrete components of the type (1.172) in the limit $\epsilon \longrightarrow 0$. The functions $h^{\mathbf{n}}(\mathbf{x})$ may therefore be used as an approximate basis in the same way as the previous basis functions $f^a(\mathbf{x}), g^b(\mathbf{x})$, with any desired accuracy depending on the choice of ϵ. It is convenient to introduce abstract bra and ket vectors associated with the basis functions $h^{\mathbf{n}}(\mathbf{x})$, denoting them by $\langle \mathbf{x}^{\mathbf{n}}|$ and $|\mathbf{x}^{\mathbf{n}}\rangle$, respectively, and writing the orthonormality relation (1.170) in bracket notation as

$$\langle \mathbf{x}^{\mathbf{n}}|\mathbf{x}^{\mathbf{n}'}\rangle \equiv \int d^3x \, h^{\mathbf{n}}(\mathbf{x})^* h^{\mathbf{n}'}(\mathbf{x}) = \delta^{\mathbf{n}\mathbf{n}'}. \tag{1.173}$$

The components $\Psi_{\mathbf{n}}(t)$ may be considered as the scalar products

$$\Psi_{\mathbf{n}}(t) \equiv \langle \mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle \approx \sqrt{\epsilon^3}\Psi(\mathbf{x}^{\mathbf{n}},t). \tag{1.174}$$

Changes of basis vectors, for instance from $|\mathbf{x}^{\mathbf{n}}\rangle$ to the states $|a\rangle$, can be performed according to the rules developed above by inserting an abstract completeness relation of the type (1.165). Thus we may expand

$$\Psi_{\mathbf{n}}(t) = \langle \mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle = \sum_{a} \langle \mathbf{x}^{\mathbf{n}}|a\rangle\langle a|\Psi(t)\rangle. \tag{1.175}$$

Also the inverse relation is true:

$$\langle a|\Psi(t)\rangle = \sum_{\mathbf{n}} \langle a|\mathbf{x}^{\mathbf{n}}\rangle\langle \mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle. \tag{1.176}$$

This is, of course, just an approximation to the integral

$$\int d^3x \, f^a(\mathbf{x})^* \langle \mathbf{x}|\Psi(t)\rangle. \tag{1.177}$$

The completeness of the basis $h^{\mathbf{n}}(\mathbf{x})$ may therefore be expressed via the abstract relation

$$\sum_{\mathbf{n}} |\mathbf{x}^{\mathbf{n}}\rangle\langle\mathbf{x}^{\mathbf{n}}| \approx 1. \tag{1.178}$$

The approximate sign turns into an equality sign in the limit of zero mesh size, $\epsilon \to 0$.

In ordinary calculus, finer and finer sums are eventually replaced by integrals. The same thing is done here. We define new continuous scalar products

$$\langle\mathbf{x}|\Psi(t)\rangle \approx \frac{1}{\sqrt{\epsilon^3}}\langle\mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle, \tag{1.179}$$

where $\mathbf{x}^{\mathbf{n}}$ are the lattice points closest to $\mathbf{x}$. With (1.174), the right-hand side is equal to $\Psi(\mathbf{x}^{\mathbf{n}},t)$. In the limit $\epsilon \to 0$, $\mathbf{x}$ and $\mathbf{x}^{\mathbf{n}}$ coincide and we have

$$\langle\mathbf{x}|\Psi(t)\rangle \equiv \Psi(\mathbf{x},t). \tag{1.180}$$

The completeness relation can be used to write

$$\begin{aligned}\langle a|\Psi(t)\rangle &\approx \sum_{\mathbf{n}}\langle a|\mathbf{x}^{\mathbf{n}}\rangle\langle\mathbf{x}^{\mathbf{n}}|\Psi(t)\rangle\\ &\approx \sum_{\mathbf{n}}\epsilon^3\langle a|\mathbf{x}\rangle\langle\mathbf{x}|\Psi(t)\rangle\Big|_{\mathbf{x}=\mathbf{x}^{\mathbf{n}}}\ ,\end{aligned} \tag{1.181}$$

which in the limit $\epsilon \to 0$ becomes

$$\langle a|\Psi(t)\rangle = \int d^3x\,\langle a|\mathbf{x}\rangle\langle\mathbf{x}|\Psi(t)\rangle. \tag{1.182}$$

This may be viewed as the result of inserting the formal completeness relation of the limiting local bra and ket basis vectors $\langle\mathbf{x}|$ and $|\mathbf{x}\rangle$,

$$\int d^3x\,|\mathbf{x}\rangle\langle\mathbf{x}| = 1, \tag{1.183}$$

evaluated between the vectors $\langle a|$ and $|\Psi(t)\rangle$.

With the limiting local basis, the wave functions can be treated as components of the state vectors $|\Psi(t)\rangle$ with respect to the local basis $|\mathbf{x}\rangle$ in the same way as any other set of components in an arbitrary basis $|a\rangle$. In fact, the expansion

$$\langle a|\Psi(t)\rangle = \int d^3x\,\langle a|\mathbf{x}\rangle\langle\mathbf{x}|\Psi(t)\rangle \tag{1.184}$$

may be viewed as a re-expansion of a component of $|\Psi(t)\rangle$ in one basis, $|a\rangle$, into those of another basis, $|\mathbf{x}\rangle$, just as in (1.164).

In order to express all these transformation properties in a most compact notation, it has become customary to deal with an arbitrary physical state vector in a *basis-independent* way and denote it by a ket vector $|\Psi(t)\rangle$. This vector may be specified in any convenient basis by multiplying it with the corresponding completeness relation

$$\sum_a |a\rangle\langle a| = 1, \tag{1.185}$$

resulting in the expansion

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle. \tag{1.186}$$

This can be multiplied with any bra vector, say $\langle b|$, from the left to obtain the expansion formula (1.166):

$$\langle b|\Psi(t)\rangle = \sum_a \langle b|a\rangle\langle a|\Psi(t)\rangle. \tag{1.187}$$

In particular, the completeness relation of the local basis states

$$\int d^3x\, |\mathbf{x}\rangle\langle\mathbf{x}| = 1 \tag{1.188}$$

leads to the expansion

$$|\Psi(t)\rangle = \int d^3x\, |\mathbf{x}\rangle\langle\mathbf{x}|\Psi(t)\rangle, \tag{1.189}$$

in which the wave function $\Psi(\mathbf{x},t) = \langle\mathbf{x}|\Psi(t)\rangle$ plays the role of an $\mathbf{x}$th component of the state vector $|\Psi(t)\rangle$ in the local basis $|\mathbf{x}\rangle$. This, in turn, is the limit of the discrete basis vectors $|\mathbf{x}^{\mathbf{n}}\rangle$,

$$|\mathbf{x}\rangle \approx \frac{1}{\sqrt{\epsilon^3}}\, |\mathbf{x}^{\mathbf{n}}\rangle\,, \tag{1.190}$$

with $\mathbf{x}^{\mathbf{n}}$ being the lattice points closest to $\mathbf{x}$.

A vector can be described equally well in bra or in ket form. To apply the above formalism consistently, we observe that the scalar products

$$\begin{aligned} \langle a|\tilde{b}\rangle &= \int d^3x\, f^a(\mathbf{x})^* \tilde{f}^b(\mathbf{x}), \\ \langle\tilde{b}|a\rangle &= \int d^3x\, \tilde{f}^b(\mathbf{x})^* f^a(\mathbf{x}) \end{aligned} \tag{1.191}$$

satisfy the identity

$$\langle\tilde{b}|a\rangle \equiv \langle a|\tilde{b}\rangle^*. \tag{1.192}$$

Therefore, when expanding a ket vector as

$$|\Psi(t)\rangle = \sum_a |a\rangle\langle a|\Psi(t)\rangle, \tag{1.193}$$

or a bra vector as

$$\langle\Psi(t)| = \sum_a \langle\Psi(t)|a\rangle\langle a|, \tag{1.194}$$

a multiplication of the first equation with the bra $\langle\mathbf{x}|$ and of the second with the ket $|\mathbf{x}\rangle$ produces equations which are complex-conjugate to each other.

Similarly, we may rewrite the nth-order term of (1.143) as

$$\begin{aligned} &\frac{1}{n!}\hat{T}\int_{t_a}^{t_b} dt_n \int_{t_a}^{t_b} dt_{n-1} \cdots \int_{t_a}^{t_b} dt_1\, \hat{H}(t_n)\hat{H}(t_{n-1})\cdots\hat{H}(t_1) \\ &= \frac{1}{n!}\hat{T}\Big(\int_{t_a}^{t_b} dt\, \hat{H}(t)\Big)^n. \end{aligned} \tag{1.195}$$

The time displacement operator $\hat{U}(t_b,t_a)$ has therefore the series expansion

$$\begin{aligned}\hat{U}(t_b,t_a) &= 1-\frac{i}{\hbar}\hat{T}\int_{t_a}^{t_b}dt\,\hat{H}(t)+\frac{1}{2!}\left(\frac{-i}{\hbar}\right)^2\hat{T}\Big(\int_{t_a}^{t_b}dt\,\hat{H}(t)\Big)^2\\ &\quad+\ldots+\frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n\hat{T}\Big(\int_{t_a}^{t_b}dt\,\hat{H}(t)\Big)^n+\ldots\,.\end{aligned}\tag{1.196}$$

The right-hand side of $\hat{T}$ contains simply the power series expansion of the exponential so that we can write

$$\hat{U}(t_b,t_a)=\hat{T}\exp\left\{-\frac{i}{\hbar}\int_{t_a}^{t_b}dt\,\hat{H}(t)\right\}.\tag{1.197}$$

If $\hat{H}$ does not depend on the time, the time-ordering operation is superfluous, the integral can be done trivially, and we recover the previous result (1.136).

1.5 Properties of Time Evolution Operator

By construction, $\hat{U}(t_b,t_a)$ has some important properties:

a) Fundamental composition law

If two time translations are performed successively, the corresponding operators $\hat{U}$ are related by

$$\hat{U}(t_b,t_a)=\hat{U}(t_b,t')\hat{U}(t',t_a),\qquad t'\in(t_a,t_b).\tag{1.198}$$

This composition law makes the operators $\hat{U}$ a representation of the abelian group of time translations. For time-independent Hamiltonians with $\hat{U}(t_b,t_a)$ given by (1.136), the proof of (1.198) is trivial. In the general case (1.197), it follows from the simple manipulation valid for $t_b>t_a$:

$$\begin{aligned}&\hat{T}\exp\left(-\frac{i}{\hbar}\int_{t'}^{t_b}\hat{H}(t)\,dt\right)\hat{T}\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t'}\hat{H}(t)\,dt\right)\\ &\quad=\hat{T}\left[\exp\left(-\frac{i}{\hbar}\int_{t'}^{t_b}\hat{H}(t)\,dt\right)\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t'}\hat{H}(t)\,dt\right)\right]\\ &\quad=\hat{T}\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t_b}\hat{H}(t)\,dt\right).\end{aligned}\tag{1.199}$$

b) Unitarity

The expression (1.197) for the time displacement operator $\hat{U}(t_b,t_a)$ was derived only for the *causal* (or *retarded*) time arguments, i.e., for t_b later than t_a. We may, however, define $\hat{U}(t_b,t_a)$ also for the *anticausal* (or *advanced*) case where t_b lies before t_a. To be consistent with the above composition law (1.198), we must have

$$\hat{U}(t_b,t_a)\equiv\hat{U}(t_a,t_b)^{-1}.\tag{1.200}$$

Indeed, when considering two states at successive times

$$|\Psi(t_a)\rangle = \hat{U}(t_a, t_b)|\Psi(t_b)\rangle, \tag{1.201}$$

the order of succession is inverted by multiplying both sides by $\hat{U}^{-1}(t_a, t_b)$:

$$|\Psi(t_b)\rangle = \hat{U}(t_a, t_b)^{-1}|\Psi(t_a)\rangle, \quad t_b < t_a. \tag{1.202}$$

The operator on the right-hand side is defined to be the time displacement operator $\hat{U}(t_b, t_a)$ from the later time t_a to the earlier time t_b.

If the Hamiltonian is independent of time, with the time displacement operator being

$$\hat{U}(t_a, t_b) = e^{-i(t_a - t_b)\hat{H}/\hbar}, \qquad t_a > t_b, \tag{1.203}$$

the unitarity of the operator $\hat{U}(t_b, t_a)$ is obvious:

$$\hat{U}^\dagger(t_b, t_a) = \hat{U}(t_b, t_a)^{-1}, \qquad t_b < t_a. \tag{1.204}$$

Let us verify this property for a general time-dependent Hamiltonian. There, a direct solution of the Schrödinger equation (1.89) for the state vector shows that the operator $\hat{U}(t_b, t_a)$ for $t_b < t_a$ has a representation just like (1.197), except for a reversed time order of its arguments. One writes this in the form [compare (1.197)]

$$\hat{U}(t_b, t_a) = \hat{\bar{T}} \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} \hat{H}(t)\, dt\right\}, \tag{1.205}$$

where $\hat{\bar{T}}$ denotes the time-antiordering operator, with an obvious definition analogous to (1.145), (1.146). This operator satisfies the relation

$$\left[\hat{T}\left(\hat{O}_1(t_1)\hat{O}_2(t_2)\right)\right]^\dagger = \hat{\bar{T}}\left(\hat{O}_2^\dagger(t_2)\hat{O}_1^\dagger(t_1)\right), \tag{1.206}$$

with an obvious generalization to the product of n operators. We can therefore conclude right away that

$$\hat{U}^\dagger(t_b, t_a) = \hat{U}(t_a, t_b), \quad t_b > t_a. \tag{1.207}$$

With $\hat{U}(t_a, t_b) \equiv \hat{U}(t_b, t_a)^{-1}$, this proves the unitarity relation (1.204), in general.

c) Schrödinger equation for $\hat{U}(t_b, t_a)$

Since the operator $\hat{U}(t_b, t_a)$ rules the relation between arbitrary wave functions at different times,

$$|\Psi(t_b)\rangle = \hat{U}(t_b, t_a)|\Psi(t_a)\rangle, \tag{1.208}$$

the Schrödinger equation (1.132) implies that the operator $\hat{U}(t_b, t_a)$ satisfies the corresponding equations

$$i\hbar\partial_t \hat{U}(t, t_a) = \hat{H}\hat{U}(t, t_a), \tag{1.209}$$

$$i\hbar\partial_t \hat{U}(t, t_a)^{-1} = -\hat{U}(t, t_a)^{-1}\hat{H}. \tag{1.210}$$

In the subsequent development, an important role will be played by the matrix elements of the time displacement operator in the localized basis states,

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) \equiv \langle \mathbf{x}_b|\hat{U}(t_b,t_a)|\mathbf{x}_a\rangle. \tag{1.211}$$

They are referred to as *time evolution* amplitudes. The functional matrix $(\mathbf{x}_b t_b|\mathbf{x}_a t_a)$ is also called the *propagator* of the system. Due to the operator equations (1.209), the propagator satisfies the Schrödinger equation

$$\left[H(-i\hbar\partial_{\mathbf{x}_b},\mathbf{x}_b,t_b) - i\hbar\partial_{t_b}\right](\mathbf{x}_b t_b|\mathbf{x}_a t_a) = 0. \tag{1.212}$$

In the quantum mechanics of nonrelativistic particles, only the propagators from earlier to later times will be relevant. It is therefore customary to introduce the so-called *causal time evolution operator* or *retarded time evolution operator*:[8]

$$\hat{U}_R(t_b,t_a) \equiv \begin{cases} \hat{U}(t_b,t_a), & t_b \ge t_a, \\ 0, & t_b < t_a, \end{cases} \tag{1.213}$$

and the associated *causal time evolution amplitude* or *retarded time evolution amplitude*

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a)_R \equiv \langle \mathbf{x}_b|\hat{U}_R(t_b,t_a)|\mathbf{x}_a\rangle. \tag{1.214}$$

Since this differs from (1.211) only for $t_b < t_a$, and since all formulas in the subsequent text will be used only for $t_b > t_a$, we shall often omit the subscript R. To abbreviate the case distinction in (1.213), it is convenient to use the *Heaviside function* defined by

$$\Theta(t) \equiv \begin{cases} 1 & t \ge 0, \\ 0 & t < 0. \end{cases}, \tag{1.215}$$

and write

$$U_R(t_b,t_a) \equiv \Theta(t_b-t_a)\hat{U}(t_b,t_a), \qquad (\mathbf{x}_b t_b|\mathbf{x}_a t_a)_R \equiv \Theta(t_b-t_a)(\mathbf{x}_b t_b|\mathbf{x}_a t_a). \tag{1.216}$$

The Heaviside function has the property that its derivative yields Dirac's δ-function

$$\partial_t\Theta(t) = \delta(t). \tag{1.217}$$

The retarded propagator satisfies the Schrödinger equation

$$\left[H(-i\hbar\partial_{\mathbf{x}_b},\mathbf{x}_b,t_b)_R - i\hbar\partial_{t_b}\right](\mathbf{x}_b t_b|\mathbf{x}_a t_a) = -i\hbar\delta(t_b-t_a)\delta^{(3)}(\mathbf{x}_b-\mathbf{x}_a). \tag{1.218}$$

The nonzero right-hand side arises from the term

$$-i\hbar\left[\partial_{t_b}\Theta(t_b-t_a)\right]\langle \mathbf{x}_b|\hat{U}(t_b,t_a)|\mathbf{x}_a\rangle = -i\hbar\delta(t_b-t_a)\langle \mathbf{x}_b|\mathbf{x}_a\rangle. \tag{1.219}$$

The δ-function on the right-hand side is the unit operator in the space of wave functions $\psi(\mathbf{x},t)$. In general, a solution of a differential operator with a unit source is called a *Green function.* Thus the causal propagator of the Schrödinger field is equal to the retarded Green function of the Schrödinger differential equation.

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[8] Compare this with the retarded *Green functions* to be introduced in Section 2.13

If the Hamiltonian does not depend on time, the propagator depends only on the time difference $t = t_b - t_a$. The causal propagator vanishes for $t < 0$. Functions $f(t)$ with this property have a characteristic Fourier transform. The integral

$$\tilde{f}(E) \equiv \int_0^\infty dt\, f(t) e^{iEt/\hbar} \tag{1.220}$$

is an analytic function in the upper half of the complex energy plane. This analyticity property is necessary and sufficient to produce a factor $\Theta(t)$ when inverting the Fourier transform via the energy integral

$$f(t) \equiv \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar}\, \tilde{f}(E) e^{-iEt/\hbar}. \tag{1.221}$$

For $t < 0$, the contour of integration may be closed by an infinite semicircle in the upper half-plane at no extra cost. Since the contour encloses no singularities, it can be contracted to a point, yielding $f(t) = 0$.

The Heaviside function $\Theta(t)$ itself is the simplest retarded function, with a Fourier representation containing only a single pole just below the origin of the complex energy plane:

$$\Theta(t) = \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{i}{E + i\eta} e^{-iEt}, \tag{1.222}$$

where η is an infinitesimally small positive number.

The retarded time evolution operator (1.213) satisfies the inhomogenous Schrödinger equation

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \hat{U}_R(t, t_a) = -i\hbar\delta(t - t_a), \tag{1.223}$$

rather than (1.209). If we define a representation independent time derivative as an abstract operator $\hat{E} \equiv i\hbar\partial_t$ acting on functions depending on an abstract time operator $\hat{t}$ with the commutation rule

$$[\hat{E}, \hat{t}] = i\hbar \tag{1.224}$$

this equation can be written as

$$(\hat{E} - \hat{H})\hat{U}_R = -i. \tag{1.225}$$

The Schrödinger equation (1.219) is recovered from this by taking the matrix elements of (1.219) between the eigenstates $|\mathbf{x}, t\}$ of space and time operators which satisfy

$$\hat{\mathbf{x}}|\mathbf{x}, t\} = \mathbf{x}|\mathbf{x}, t\}, \qquad \hat{t}|\mathbf{x}, t\} = t|\mathbf{x}, t\}, \tag{1.226}$$

and

$$\{\mathbf{x}, t|\hat{p} = -i\frac{\partial}{\partial \mathbf{x}}\{\mathbf{x}, t|, \qquad \{\mathbf{x}, t|\hat{E} = i\frac{\partial}{\partial t}\{\mathbf{x}, t|. \tag{1.227}$$

For a free particle with a Hamilton operator $\hat{H} = \hat{\mathbf{p}}^2/2M$, the spectrum is completely continuous. The eigenfunctions are (1.120) with energies $E(\mathbf{p}) = \mathbf{p}^2/2M$. Inserting the completeness relation (1.118) into Eq. (1.211) with the operator (1.203), we obtain the time evolution amplitude for a free particle

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \int \frac{d^D p}{(2\pi\hbar)^D} \exp\left\{\frac{i}{\hbar}\left[\mathbf{p}(\mathbf{x}_b - \mathbf{x}_a) - \frac{\mathbf{p}^2}{2M}(t_b - t_a)\right]\right\}. \tag{1.228}$$

The momentum integrals can easily be done. First we perform a quadratic completion in the exponent and rewrite it as

$$i\mathbf{p}(\mathbf{x}_b - \mathbf{x}_a) - \frac{i\hbar}{2M}\mathbf{p}^2(t_b - t_a) = \frac{i\hbar}{2M}\left(\mathbf{p} - \frac{1}{M}\frac{\mathbf{x}_b - \mathbf{x}_a}{t_b - t_a}\right)(t_b - t_a) + \frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a}. \tag{1.229}$$

Then we replace the integration variables by the shifted momenta $\mathbf{p}' = \mathbf{p} - (\mathbf{x}_b - \mathbf{x}_a)/(t_b - t_a)M$, and the amplitude (1.228) becomes

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = F(t_b - t_a) \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{x}_b - \mathbf{x}_a)^2}{t_b - t_a}\right], \tag{1.230}$$

where $F(t_b - t_a)$ is the integral over the shifted momenta

$$F(t_b - t_a) \equiv \int \frac{d^D p'}{(2\pi\hbar)^D} \exp\left\{\frac{i}{\hbar}\left[\mathbf{p}'(\mathbf{x}_b - \mathbf{x}_a) - \frac{\mathbf{p}'^2}{2M}(t_b - t_a)\right]\right\}. \tag{1.231}$$

This can be performed using the *Fresnel integral formula*

$$\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \exp\left(i\frac{a}{2}p^2\right) = \frac{1}{\sqrt{|a|}}\left\{\begin{array}{ll} \sqrt{i}, & a > 0, \\ 1/\sqrt{i}, & a < 0. \end{array}\right. \tag{1.232}$$

Here the square root $\sqrt{i}$ denotes the phase factor $e^{i\pi/4}$: This follows from the Gauss formula

$$\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \exp\left(-\frac{\alpha}{2}p^2\right) = \frac{1}{\sqrt{\alpha}}, \qquad \mathrm{Re}\,\alpha > 0, \tag{1.233}$$

by continuing α analytically from positive values into the right complex half-plane. As long as $\mathrm{Re}\,\alpha > 0$, this is straightforward. On the boundaries, i.e., on the positive and negative imaginary axes, one has to be careful. At $\alpha = \pm ia + \eta$ with $a \gtrless 0$ and infinitesimal $\eta > 0$, the integral is certainly convergent yielding (1.232). But the integral also converges for $\eta = 0$, as can easily be seen by substituting $x^2 = z$.

Since the Fresnel formula is a special analytically continued case of the Gauss formula, we shall in the sequel always speak of Gaussian integrations and use Fresnel's name only if the imaginary nature of the quadratic exponent is to be emphasized.

Applying this formula to (1.231), we obtain

$$F(t_b - t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b - t_a)/M}^{\,D}}, \tag{1.234}$$

so that the full time evolution amplitude of a free massive point particle is, for each Cartesian component

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}^D} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{t_b-t_a}\right]. \tag{1.235}$$

In the limit $t_b \to t_a$, the left-hand side becomes the scalar product $\langle\mathbf{x}_b|\mathbf{x}_a\rangle = \delta^{(D)}(\mathbf{x}_b-\mathbf{x}_a)$, implying the following limiting formula for the δ-function

$$\delta^{(D)}(\mathbf{x}_b-\mathbf{x}_a) = \lim_{t_b-t_a\to 0} \frac{1}{\sqrt{2\pi i\hbar(t_b-t_a)/M}^D} \exp\left[\frac{i}{\hbar}\frac{M}{2}\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{t_b-t_a}\right]. \tag{1.236}$$

1.6 Heisenberg Picture of Quantum Mechanics

The unitary time displacement operator $\hat{U}(t,t_a)$ may be used to give a different formulation of quantum mechanics bearing the closest resemblance to classical mechanics. This formulation, called the *Heisenberg picture*, derives from the postulate that the transition from classical to quantum mechanics can be achieved by replacing the canonical variables $p_i(t)$ and $q_i(t)$ in phase space by *matrices*, denoted by $p_{Hi}(t)$, $q_{Hi}(t)$. The Heisenberg postulate is applicable only as long as the canonical quantization rules are valid requiring that q_i be Cartesian coordinates. To indicate this, we prefer using the letter x for the position variable, as in Section 1.3, the corresponding Heisenberg matrix being $x_H(t)$.

The Heisenberg matrices turn out to be subject to the same equations of motion as the classical quantities, except that Poisson brackets are replaced by $i/\hbar$ times the matrix commutators at equal times. This implies the fundamental Poisson brackets to turn into the canonical matrix commutation rules at equal times. Suppressing the subscripts i, these read

$$\begin{aligned} [\hat{p}_H(t),\hat{x}_H(t)] &= -i\hbar, \\ [\hat{p}_H(t),\hat{p}_H(t)] &= 0, \\ [\hat{x}_H(t),\hat{x}_H(t)] &= 0. \end{aligned} \tag{1.237}$$

The fundamental Hamilton equations of motion of classical mechanics turn into the Heisenberg equations of motion

$$\begin{aligned} \dot{\hat{p}}_H(t) &= \frac{i}{\hbar}\left[\hat{H}_H,\hat{p}_H(t)\right], \\ \dot{\hat{x}}_H(t) &= \frac{i}{\hbar}\left[\hat{H}_H,\hat{x}_H(t)\right], \end{aligned} \tag{1.238}$$

where

$$\hat{H}_H \equiv H(\hat{p}_H(t),\hat{x}_H(t),t) \tag{1.239}$$

is the Hamiltonian in the Heisenberg picture. Similarly, the Heisenberg equation of motion for arbitrary observable function $O(p_i(t), x_i(t), t)$ goes over into the matrix commutator equation for the Heisenberg operator

$$\hat{O}_H(t) \equiv O(\hat{p}_H(t), \hat{x}_H(t), t), \tag{1.240}$$

namely,

$$\frac{d}{dt}\hat{O}_H = \frac{i}{\hbar}[\hat{H}_H, \hat{O}_H] + \frac{\partial}{\partial t}\hat{O}_H. \tag{1.241}$$

These rules are referred to as *Heisenberg's correspondence principle.*

The relation between Schrödinger's and Heisenberg's picture is supplied by the time displacement operator. Let $\hat{O}$ be an arbitrary observable in the Schrödinger description

$$\hat{O}(t) \equiv O(\hat{p}, \hat{x}, t). \tag{1.242}$$

If $|\Psi(t)\rangle$ is an arbitrary complete set of solutions of the Schrödinger equation, the operator $\hat{O}$ can be specified in terms of its matrix elements

$$O_{ab}(t) \equiv \langle \Psi_a(t)|\hat{O}(t)|\Psi_b(t)\rangle. \tag{1.243}$$

We can now use the unitary operator $\hat{U}(t, t_a)$ to go to a new time-independent basis $|\Psi_a\rangle$, defined by

$$|\Psi_a(t)\rangle \equiv \hat{U}(t, t_a)|\Psi_a\rangle, \tag{1.244}$$

where t_a is some arbitrary but fixed time. Simultaneously, we transform the Schrödinger operators of the canonical coordinates $\hat{p}$ and $\hat{x}$ into the time-dependent canonical *Heisenberg operators* $\hat{p}_H(t)$ and $\hat{x}_H(t)$ via

$$\begin{aligned} \hat{p}_H(t) &\equiv \hat{U}(t, t_a)^{-1}\, \hat{p}\, \hat{U}(t, t_a), \\ \hat{x}_H(t) &\equiv \hat{U}(t, t_a)^{-1}\, \hat{x}\, \hat{U}(t, t_a). \end{aligned} \tag{1.245}$$

At the time t_a, the Heisenberg operators $\hat{p}_H(t)$ and $\hat{x}_H(t)$ coincide with $\hat{p}$ and $\hat{x}$, respectively. Likewise, an arbitrary observable $\hat{O}(t)$ is transformed into the associated Heisenberg operator:

$$\begin{aligned} \hat{O}_H(t) &\equiv \hat{U}(t, t_a)^{-1} O(\hat{p}, \hat{x}, t) \hat{U}(t, t_a) \\ &\equiv O\left(\hat{p}_H(t), \hat{x}_H(t), t\right). \end{aligned} \tag{1.246}$$

The Heisenberg matrices $O_H(t)$ are then obtained from the Heisenberg operators $\hat{O}_H(t)$ by sandwiching them between any convenient choice of complete basis vectors with no time dependence $|\Psi_b\rangle$, i.e., the matrix elements of $O_H(t)$ are given by

$$O_H(t)_{ab} \equiv \langle \Psi_a|\hat{O}_H(t)|\Psi_b\rangle. \tag{1.247}$$

Note that the time dependence of these matrix elements is completely due to the time dependence of the operators,

$$\frac{d}{dt}O_H(t)_{ab} \equiv \langle \Psi_a|\frac{d}{dt}\hat{O}_H(t)|\Psi_b\rangle. \tag{1.248}$$

This is in contrast to the Schrödinger representation (1.243), where the right-hand side would have contained two more terms from the time dependence of the wave functions. Due to the absence of such terms in (1.248) it is possible to study the equation of motion of the Heisenberg matrices independently of the basis by considering directly the Heisenberg operators. It is straightforward to verify that they do indeed satisfy the rules of Heisenberg's correspondence principle. Consider the time derivative of an arbitrary observable $\hat{O}_H(t)$,

$$\begin{aligned}\frac{d}{dt}\hat{O}_H(t) &= \left(\frac{d}{dt}\hat{U}^{-1}(t,t_a)\right)\hat{O}(t)\hat{U}(t,t_a)\\ &+ \hat{U}^{-1}(t,t_a)\left(\frac{\partial}{\partial t}\hat{O}(t)\right)\hat{U}(t,t_a)+\hat{U}^{-1}(t,t_a)\hat{O}(t)\left(\frac{d}{dt}\hat{U}(t,t_a)\right),\end{aligned}$$

which can be rearranged as

$$\begin{aligned}&\left[\left(\frac{d}{dt}\hat{U}^{-1}(t,t_a)\right)\hat{U}(t,t_a)\right]\hat{U}^{-1}(t,t_a)\hat{O}(t)\hat{U}(t,t_a) \qquad (1.249)\\ &+\left[\hat{U}^{-1}(t,t_a)\hat{O}(t)\hat{U}(t,t_a)\right]\hat{U}^{-1}(t,t_a)\frac{d}{dt}\hat{U}(t,t_a)+\hat{U}^{-1}(t,t_a)\left(\frac{\partial}{\partial t}\hat{O}(t)\right)\hat{U}(t,t_a).\end{aligned}$$

Using (1.209), we obtain

$$\frac{d}{dt}\hat{O}_H(t)=\frac{i}{\hbar}\left[\hat{U}^{-1}\hat{H}\hat{U},\hat{O}_H\right]+\hat{U}^{-1}\left(\frac{\partial}{\partial t}\hat{O}(t)\right)\hat{U}. \qquad (1.250)$$

After inserting (1.246), we find the equation of motion for the Heisenberg operator:

$$\frac{d}{dt}\hat{O}_H(t)=\frac{i}{\hbar}\left[\hat{H}_H,\hat{O}_H(t)\right]+\left(\frac{\partial}{\partial t}\hat{O}\right)_H(t). \qquad (1.251)$$

By sandwiching this equation between the complete time-independent basis states $|\Psi_a\rangle$ in the Hilbert space, it holds for the matrices and turns into the Heisenberg equation of motion. For the phase space variables $p_H(t)$, $x_H(t)$ themselves, these equations reduce, of course, to the Hamilton equations of motion (1.238)..

Thus we have shown that Heisenberg's matrix quantum mechanics is completely equivalent to Schrödinger's and that the Heisenberg matrices obey the same Hamilton equations as the classical observables.

1.7 Classical and Quantum Statistics

Consider a physical system with a constant number of particles N whose Hamiltonian has no explicit time dependence. If it is brought in contact with a thermal reservoir at a temperature T and has reached equilibrium, its thermodynamic properties can be obtained through the following rules: At the level of classical mechanics, each volume element in phase space

$$\frac{dp\,dq}{h}=\frac{dp\,dq}{2\pi\hbar} \qquad (1.252)$$

is occupied with a probability proportional to the *Boltzmann factor*

$$e^{-H(p,q)/k_BT}, \tag{1.253}$$

where k_B is the *Boltzmann constant*

$$k_B = 1.3806221(59) \times 10^{-16}\,\text{erg/Kelvin}. \tag{1.254}$$

The number in parentheses indicates the experimental uncertainty of the two digits in front of it. The quantity $1/k_BT$ has the dimension of an inverse energy and is commonly denoted by β. It will be called the *inverse temperature*, forgetting about the factor k_B. In fact, we shall sometimes take T to be measured in energy units k_B times Kelvin rather than in Kelvin. Then we may drop k_B in all formulas.

The integral over the Boltzmann factors of all phase space elements,[9]

$$Z_{\text{cl}}(T) \equiv \int \frac{dp\,dq}{2\pi\hbar}\, e^{-H(p,q)/k_BT}, \tag{1.255}$$

is called the *classical partition function*. It contains all classical thermodynamic information of the system. Of course, for a general Hamiltonian system with many degrees of freedom, the phase space integral is $\prod_n \int dp_n\, dq_n/2\pi\hbar$. The normalized Boltzmann factor

$$w(p,q) = Z_{\text{cl}}^{-1}(T)e^{-H(p,q)/k_BT} \tag{1.256}$$

is called the *classical Gibbs distribution function*.

In quantum statistics, the Hamiltonian is replaced by the operator $\hat{H}$ and the integral over phase space by the trace in the Hilbert space. This leads to the *quantum-statistical partition function*

$$Z(T) \equiv \text{Tr}\left(e^{-\hat{H}/k_BT}\right) \equiv \text{Tr}\left(e^{-H(\hat{p},\hat{x})/k_BT}\right), \tag{1.257}$$

where $\text{Tr}\,\hat{O}$ denotes the trace of the operator $\hat{O}$. If $|n\rangle$ are eigenstates of the Hamiltonian with energy E_n, the partition function becomes a sum

$$Z(T) = \sum_n e^{-E_n/k_BT} \tag{1.258}$$

The normalized Boltzmann factor

$$w_n = Z_{\text{cl}}^{-1}(T)e^{-E_n/k_BT} \tag{1.259}$$

is called the *quantum statistical Gibbs distribution function*.

The right-hand side contains the position operator $\hat{x}$ in Cartesian coordinates rather than $\hat{q}$ to ensure that the system can be quantized canonically. In cases such as the spinning top, the trace formula is also valid but the Hilbert space is spanned by the representation states of the angular momentum operators. In more general Lagrangian systems, the quantization has to be performed differently in the way to be described in Chapters 10 and 11.

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[9] In the sequel we shall always work at a fixed volume V and therefore suppress the argument V everywhere.

At this point we make an important observation: The quantum partition function is related in a very simple way to the quantum-mechanical time displacement operator. To emphasize this relation we shall define the trace of this operator as the *quantum-mechanical partition function*:

$$Z_{\rm QM}(t_b, t_a) \equiv {\rm Tr}\left(\hat{U}(t_b, t_a)\right) = {\rm Tr}\left(e^{-i(t_b-t_a)\hat{H}/\hbar}\right). \tag{1.260}$$

This may be considered as the partition function associated with a "quantum-mechanical Gibbs distribution"

$$w_n = Z_{\rm QM}^{-1}(t_b - t_a)e^{iE_n(t_b-t_a)/\hbar}. \tag{1.261}$$

Obviously, the quantum-statistical partition function $Z(T)$ may be obtained from the quantum-mechanical one by continuing the time interval $t_b - t_a$ to the negative imaginary value

$$t_b - t_a = -\frac{i\hbar}{k_B T} \equiv -i\hbar\beta. \tag{1.262}$$

This simple formal relation shows that the trace of the time evolution operator contains all information on the thermodynamic equilibrium properties of a quantum system.

For general systems containing many bodies it is often convenient to study their equilibrium properties in contact with a particle reservoir characterized by a chemical potential μ. For this one defines what is called the *grand-canonical quantum-statistical partition function*

$$Z_G(T, \mu) = {\rm Tr}\left(e^{-(\hat{H}-\mu\hat{N})/k_B T}\right). \tag{1.263}$$

Here $\hat{N}$ is the operator counting the number of particles in each state of the ensemble. The combination of operators in the exponent,

$$\hat{H}_G = \hat{H} - \mu\hat{N}, \tag{1.264}$$

is called the *grand-canonical Hamiltonian.*

Given a partition function $Z(T)$ at a fixed particle number N, the *free energy* is defined by

$$F(T) = -k_B T \log Z(T). \tag{1.265}$$

Its grand-canonical version at a fixed chemical potential is

$$F_G(T, \mu) = -k_B T \log Z_G(T, \mu). \tag{1.266}$$

The *average energy* or *internal energy* is defined by

$$E = {\rm Tr}\left(\hat{H}e^{-\hat{H}/k_B T}\right) \Big/ {\rm Tr}\left(e^{-\hat{H}/k_B T}\right). \tag{1.267}$$

It may be obtained from the partition function $Z(T)$ by forming the temperature derivative

$$E = Z^{-1} k_B T^2 \frac{\partial}{\partial T} Z(T) = k_B T^2 \frac{\partial}{\partial T} \log Z(T). \tag{1.268}$$

In terms of the free energy (1.265), this becomes

$$E = \left(1 - T\frac{\partial}{\partial T}\right) F(T) \tag{1.269}$$

For a grand-canonical ensemble we may introduce an *average particle number* defined by

$$N = \mathrm{Tr}\left(\hat{N} e^{-(\hat{H}-\mu\hat{N})/k_B T}\right) / \mathrm{Tr}\left(e^{-(\hat{H}-\mu\hat{N})/k_B T}\right). \tag{1.270}$$

This can be derived from the grand-canonical partition function as

$$N = Z_G{}^{-1}(T,\mu) k_B T \frac{\partial}{\partial \mu} Z_G(T,\mu) = k_B T \frac{\partial}{\partial \mu} \log Z_G(T,\mu), \tag{1.271}$$

or, using the grand-canonical free energy, as

$$N = -\frac{\partial}{\partial \mu} F_G(T,\mu). \tag{1.272}$$

The average energy in a grand-canonical system,

$$E = \mathrm{Tr}\left(\hat{H} e^{-(\hat{H}-\mu\hat{N})/k_B T}\right) / \mathrm{Tr}\left(e^{-(\hat{H}-\mu\hat{N})/k_B T}\right), \tag{1.273}$$

can be obtained by forming, in analogy with (1.268) and (1.269), the derivative

$$\begin{aligned} E - \mu N &= Z_G{}^{-1}(T,\mu) k_B T^2 \\ &= \left(1 - T\frac{\partial}{\partial T}\right) F_G(T,\mu). \end{aligned} \tag{1.274}$$

In thermodynamic considerations, a quantity of fundamental interest is the *entropy*. To define it, let us calculate the partition function

$$Z(T) = \mathrm{Tr}\left(e^{-\hat{H}/k_B T}\right) \tag{1.275}$$

in terms of all eigenstates $|n\rangle$ of the Hamiltonian, i.e.

$$Z(T) = \sum_n e^{-E_n/k_B T}. \tag{1.276}$$

This can be rewritten as an integral

$$Z(T) = \int d\varepsilon\, \rho(\varepsilon) e^{-\varepsilon/k_B T}, \tag{1.277}$$

with

$$\rho(\varepsilon) = \sum_n \delta(\varepsilon - E_n) \tag{1.278}$$

being the density of states available to the system in the energy interval $(\varepsilon, \varepsilon + d\varepsilon)$. The density may also be written formally as

$$\rho(\varepsilon) = \mathrm{Tr}\, \delta(\varepsilon - \hat{H}). \tag{1.279}$$

The integral

$$N(E) = \int_0^E d\varepsilon\, \rho(\varepsilon) \tag{1.280}$$

is the number of states up to energy E. For a large number of particles, the density is a rapidly growing function of energy. For a system of N free particles, for example, the number of states up to energy E is given by

$$N(E) = \sum_{\mathbf{p}_i} \Theta(E - \sum_{i=1}^{N} \mathbf{p}_i^2/2M), \tag{1.281}$$

where each of the particle momenta $\mathbf{p}_i$ is summed over all discrete momenta $\mathbf{p}^{\mathbf{m}}$ in (1.110) available to a single particle in a finite box of volume $V = L^3$. For a large V, the sum can be converted into an integral[10]

$$N(E) = V^N \prod_{i=1}^{N} \left[\int \frac{d^3 p_i}{(2\pi\hbar)^3} \right] \Theta(E - \sum_{i=1}^{N} \mathbf{p}_i^2/2M), \tag{1.282}$$

which is simply $\left[V/(2\pi\hbar)^3\right]^N$ times the volume Ω_{3N} of a $3N$-dimensional sphere of radius $\sqrt{2ME}$:[11]

$$\begin{aligned} N(E) &= \left[\frac{V}{(2\pi\hbar)^3}\right]^N \Omega_{3N} \\ &\equiv \left[\frac{V}{(2\pi\hbar)^3}\right]^N \frac{(2\pi ME)^{3N/2}}{\Gamma(\frac{3}{2}N+1)}. \end{aligned} \tag{1.283}$$

Therefore, the density $\rho = \partial N/\partial E$ is given by

$$\rho(E) = \left[\frac{V}{(2\pi\hbar)^3}\right]^N 2\pi M \frac{(2\pi ME)^{3N/2-1}}{\Gamma(\frac{3}{2}N)}. \tag{1.284}$$

It grows with the very large power $E^{3N/2}$ in the energy. Nevertheless, the integral for the partition function (1.277) is convergent, due to the overwhelming exponential falloff of the Boltzmann factor, e^{-E/k_BT}. As the two functions $\rho(e)$ and e^{-e/k_BT} are multiplied with each other, the result is a function which peaks very sharply at the average energy E of the system. The position of the peak depends on the temperature T. For the free N particle system, for example,

$$\rho(\varepsilon) e^{-\varepsilon/k_BT} \sim e^{(3N/2-1)\log\varepsilon - \varepsilon/k_BT}. \tag{1.285}$$

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[10] Remember, however, the exception noted in the footnote to Eq. (1.115) for systems possessing a condensate.

[11] The surface of a sphere of radius R in D dimensions is $2\pi^{D/2}R^{D-1}/\Gamma(D/2)$, the volume is $\Omega_D = R/D\times$ surface $= \pi^{D/2}R^D/\Gamma(D/2+1)$.

This function has a sharp peak at

$$\varepsilon = E(T) = k_BT\left(\frac{3N}{2}-1\right) \approx k_BT\frac{3N}{2}. \tag{1.286}$$

The width of the peak is found by expanding (1.285) in $\delta\varepsilon = \varepsilon - E(T)$:

$$\exp\left\{\frac{3N}{2}\log E(T) - \frac{E(T)}{k_BT} - \frac{1}{2E^2(T)}\frac{3N}{2}(\delta\varepsilon)^2 + \dots\right\}. \tag{1.287}$$

Thus, as soon as $\delta\varepsilon$ gets to be of the order of $E(T)/\sqrt{N}$, the exponential is reduced by a factor two with respect to $E(T) \approx k_BT\,3N/2$. The deviation is of a relative order $1/\sqrt{N}$, i.e., the peak is very sharp. With N being very large, the peak at $E(T)$ of width $E(T)/\sqrt{N}$ can be idealized by a δ-function, and we may write

$$\rho(\varepsilon)e^{-\varepsilon/k_BT} \approx \delta(\varepsilon - E(T))N(T)e^{-E(T)/k_BT}. \tag{1.288}$$

The quantity $N(T)$ measures the total number of states over which the system is distributed at the temperature T.

The entropy $S(T)$ is now defined in terms of $N(T)$ by

$$N(T) = e^{S(T)/k_B}. \tag{1.289}$$

Inserting this with (1.288) into (1.277), we see that in the limit of a large number of particles N:

$$Z(T) = e^{-[E(T)-TS(T)]/k_BT}. \tag{1.290}$$

Using (1.265), the free energy can thus be expressed in the form

$$F(T) = E(T) - TS(T). \tag{1.291}$$

By comparison with (1.269) we see that the entropy may be obtained from the free energy directly as

$$S(T) = -\frac{\partial}{\partial T}F(T). \tag{1.292}$$

For grand-canonical ensembles we may similarly consider

$$Z_G(T,\mu) = \int d\varepsilon\, dn\, \rho(\varepsilon,n)e^{-(\varepsilon-\mu n)/k_BT}, \tag{1.293}$$

where

$$\rho(\varepsilon,n)e^{-(\varepsilon-\mu n)/k_BT} \tag{1.294}$$

is now strongly peaked at $\varepsilon = E(T,\mu)$, $n = N(T,\mu)$ and can be written approximately as

$$\begin{aligned}\rho(\varepsilon,n)e^{-(\varepsilon-\mu n)/k_BT} &\approx \delta\left(\varepsilon - E(T,\mu)\right)\delta\left(n - N(T,\mu)\right)\\ &\quad\times e^{S(T,\mu)/k_B}e^{-[E(T,\mu)-\mu N(T,\mu)]/k_BT}.\end{aligned} \tag{1.295}$$

Inserting this back into (1.293) we find for large N

$$Z_G(T,\mu) = e^{-[E(T,\mu)-\mu N(T,\mu)-TS(T,\mu)]/k_BT}. \tag{1.296}$$

For the grand-canonical free energy (1.266), this implies the relation

$$F_G(T,\mu) = E(T,\mu) - \mu N(T,\mu) - TS(T,\mu). \tag{1.297}$$

By comparison with (1.274) we see that the entropy can be calculated directly from the derivative of the grand-canonical free energy

$$S(T,\mu) = -\frac{\partial}{\partial T} F_G(T,\mu). \tag{1.298}$$

The particle number is, of course, found from the derivative (1.272) with respect to the chemical potential, as follows directly from the definition (1.293).

The canonical free energy and the entropy appearing in the above equations depend on the particle number N and the volume V of the system, i.e., they are more explicitly written as $F(T,N,V)$ and $S(T,N,V)$, respectively.

In the arguments of the grand-canonical quantities, the particle number N is replaced by the chemical potential μ.

Among the arguments of the grand-canonical energy $F_G(T,\mu,V)$, the volume V is the only one which grows with the system. Thus $F_G(T,\mu,V)$ must be directly proportional to V. The proportionality constant defines the *pressure* p of the system:

$$F_G(T,\mu,V) \equiv -p(T,\mu,V)V. \tag{1.299}$$

Under infinitesimal changes of the three variables, $F_G(T,\mu,V)$ changes as follows:

$$dF_G(T,\mu,V) = -SdT + \mu dN - pdV. \tag{1.300}$$

The first two terms on the right-hand side follow from varying Eq. (1.297) at a fixed volume. When varying the volume, the definition (1.299) renders the last term.

Inserting (1.299) into (1.297), we find *Eulers relation*:

$$E = TS + \mu N - pV, \tag{1.301}$$

The energy has S, N, V as natural variables. Equivalently, we may write

$$F = -\mu N - pV, \tag{1.302}$$

where T, N, V are the natural variables.

Notes and References

For more details see some standard textbooks:

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2

Field Formulation of Many-Body Quantum Physics

A sample of material composed of a large number of microscopic particles is called a *many-body system*. The microscopic particles may either be all identical or of different species. Examples are crystal lattices, liquids, and gases, all of these being aggregates of molecules and atoms. Molecules are composed of atoms which, in turn, consist of an atomic nucleus and electrons, held together by electromagnetic forces, or more precisely their quanta, the photons. The mass of an atom is mostly due to the nucleus, only a small fraction being due to the electrons and an even smaller fraction due to the electromagnetic binding energy. Atomic nuclei are themselves bound states of nucleons, held together by mesonic forces, or more precisely their quanta, the mesons. The nucleons and mesons, finally, consist of the presently most fundamental objects of nuclear material, called quarks, held together by gluonic forces. Quarks and gluons are apparently as fundamental as electrons and photons. It is a wonderful miracle of nature that this deep hierarchy of increasingly fundamental particles allows for a common description with the help of a single theoretical structure called quantum field theory.

As a first step towards developing this powerful theory we shall start from the well-founded Schrödinger theory of nonrelativistic spinless particles. We show that there exists a completely equivalent formulation of this theory in terms of quantum fields. This formulation will serve as a basis for setting up various quantum field theoretical models which can eventually be composed to explain the physics of the entire particle hierarchy described above.

2.1 Mechanics and Quantum Mechanics for n Distinguishable Nonrelativistic Particles

For a many-body system with only one type of nonrelativistic spinless particles of mass M, which may be spherical atoms or molecules, the classical Lagrangian has the form

$$L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t) = \sum_{\nu=1}^{n} \frac{M}{2}\dot{\mathbf{x}}_\nu^2 - V(\mathbf{x}_1, \dots, \mathbf{x}_n; t), \tag{2.1}$$

where the arguments $\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu$ in $L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t)$ stand, pars pro toto, for all positions $\mathbf{x}_\nu$ and velocities $\dot{\mathbf{x}}_\nu$, $\nu = 1, \dots, n$. The general n-body potential $V(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ can usually be assumed to consist of a sum of an *external potential* $V_1(\mathbf{x}_\nu; t)$ and a *pair potential* $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$, also called *one-* and *two-body* or *pair potentials*, respectively:

$$V(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = \sum_\nu V_1(\mathbf{x}_\nu; t) + \frac{1}{2} \sum_{\nu,\mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \tag{2.2}$$

The second sum is symmetric in μ and ν, so that $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ may be taken as a symmetric function of the two spatial arguments—any asymmetric part would not contribute. The symmetry ensures the validity of *Newton's third principle* "actio equal reactio". The two-body potential is initially defined only for $\mu \neq \nu$, and the sum is restricted accordingly, but for the development to come it will be useful to include also the $\mu = \nu$ -terms into the second sum (2.2), and compensate this by an appropriate modification of the one-body potential $V_1(\mathbf{x}_\nu; t)$, so that the total potential remains the same. Such a rearrangement excludes pair potentials $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ which are singular at the origin, such as the Coulomb potential between point charges $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) = e^2/4\pi|\mathbf{x}_\nu - \mathbf{x}_\mu|$. Physically, this is not a serious obstacle since all charges in nature have really a finite charge radius. Even the light fundamental particles electrons and muons possess a finite charge radius, as will be seen in Chapter 10.

At first we shall consider all particles to be distinguishable. This often unphysical assumption will be removed later.

The Euler-Lagrange equations of motion associated with the above Lagrangian read

$$M\ddot{\mathbf{x}}_\nu = -\frac{\partial V_1(\mathbf{x}_\nu; t)}{\partial \mathbf{x}_\nu} - \sum_\mu \frac{\partial}{\partial \mathbf{x}_\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \tag{2.3}$$

The transition to the Hamiltonian formalism proceeds by introducing the canonical momenta

$$\mathbf{p}_\nu = \frac{\partial L}{\partial \dot{\mathbf{x}}_\nu} = M\dot{\mathbf{x}}_\nu \tag{2.4}$$

and calculating the Legendre transform

$$\begin{aligned} H(\mathbf{p}_\nu, \mathbf{x}_\nu; t) &= \left[\sum_\nu \mathbf{p}_\nu \dot{\mathbf{x}}_\nu - L(\mathbf{x}_\nu, \dot{\mathbf{x}}_\nu; t)\right]_{\dot{\mathbf{x}}_\nu = \mathbf{p}_\nu/M} \\ &= \sum_\nu \frac{\mathbf{p}_\nu^2}{2M} + \sum_\nu V_1(\mathbf{x}_\nu; t) + \frac{1}{2}\sum_{\nu,\mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t). \end{aligned} \tag{2.5}$$

The Hamilton equations of motions are

$$\begin{aligned} \dot{\mathbf{p}}_\nu = \{H, \mathbf{p}_\nu\} &= -\frac{\partial V_1(\mathbf{x}_\nu; t)}{\partial \mathbf{x}_\nu} - \sum_\mu \frac{\partial}{\partial \mathbf{x}_\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t), \\ \dot{\mathbf{x}}_\nu = \{H, \mathbf{x}_\nu\} &= \frac{\partial H}{\partial \mathbf{p}_\nu} = \frac{\mathbf{p}_\nu}{M}, \end{aligned} \tag{2.6}$$

with the Poisson brackets

$$\{A,B\} = \sum_{\nu=1}^{n} \left(\frac{\partial A}{\partial \mathbf{p}_\nu} \frac{\partial B}{\partial \mathbf{x}_\nu} - \frac{\partial B}{\partial \mathbf{p}_\nu} \frac{\partial A}{\partial \mathbf{x}_\nu} \right). \tag{2.7}$$

An arbitrary observable $F(\mathbf{p}_\nu, \mathbf{x}_\nu; t)$ changes as a function of time according to the equation of motion

$$\frac{dF}{dt} = \{H,F\} + \frac{\partial F}{\partial t}. \tag{2.8}$$

It is now straightforward to write down the laws of quantum mechanics for the system. We follow the rules in Eqs. (1.132)–(1.134), and take the local basis

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \tag{2.9}$$

as eigenstates of the position operators $\hat{\mathbf{x}}_\nu$:

$$\hat{\mathbf{x}}_\nu |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle = \mathbf{x}_\nu |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle, \quad \nu = 1, \dots, n. \tag{2.10}$$

They are orthonormal to each other,

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \mathbf{x}'_1, \dots, \mathbf{x}'_n \rangle = \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_n), \tag{2.11}$$

and form a complete basis in the space of localized n-particle states:

$$\int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle\langle \mathbf{x}_1, \dots, \mathbf{x}_n| = 1. \tag{2.12}$$

An arbitrary state is denoted by a ket vector and can be expanded in this basis by multiplying the state formally with the unit operator (2.12), yielding the expansion

$$|\psi(t)\rangle \;\equiv\; 1 \times |\psi(t)\rangle = \int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle\langle \mathbf{x}_1, \dots, \mathbf{x}_n|\psi(t)\rangle. \tag{2.13}$$

The scalar products

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \psi(t)\rangle \equiv \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \tag{2.14}$$

are the wave functions of the n-body system. They are the probability amplitudes for the particle 1 to be found at $\mathbf{x}_1$, particle 2 at $\mathbf{x}_2$, etc..

The Schrödinger equation reads, in operator form

$$\hat{H}|\psi(t)\rangle = H(\hat{\mathbf{p}}_\nu, \hat{\mathbf{x}}_\nu; t)|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \tag{2.15}$$

where $\hat{\mathbf{p}}_\nu$ are Schrödinger's momentum operators, whose action upon the wave functions is specified by the rule

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_n | \hat{\mathbf{p}}_\nu = -i\hbar\partial_{\mathbf{x}_\nu} \langle \mathbf{x}_1, \dots, \mathbf{x}_n|. \tag{2.16}$$

Multiplication of (2.15) from the left with the bra vectors $\langle \mathbf{x}_1, \dots, \mathbf{x}_n|$ yields via (2.16) the Schrödinger differential equation for the wave functions:

$$\begin{aligned} & H(-i\hbar\partial_{\mathbf{x}_\nu}, \mathbf{x}_\nu; t)\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \\ &= \left[-\sum_\nu \frac{\hbar^2}{2M}\partial^2_{\mathbf{x}_\nu} + \sum_\nu V_1(\mathbf{x}_\nu; t) + \frac{1}{2}\sum_{\nu,\mu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)\right] \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) \\ &= i\hbar\partial_t\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \end{aligned} \tag{2.17}$$

In many physical systems, the potentials $V_1(\mathbf{x}_\nu; t)$ and $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$ are independent of time. Then we can factor out the time dependence of the wave functions with fixed energy as

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = e^{-iEt/\hbar}\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n), \tag{2.18}$$

and find for $\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n)$ the time-independent Schrödinger equation

$$H(-i\hbar\partial_{\mathbf{x}_\nu}, \mathbf{x}_\nu; t)\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n) = E\psi_E(\mathbf{x}_1, \dots, \mathbf{x}_n). \tag{2.19}$$

2.2 Identical Particles — Bosons and Fermions

The quantum mechanical rules presented in the last section were written down under the assumption that all particles are distinguishable. For a realistic n-body system, however, this is an unphysical assumption. For example, there is no way of distinguishing the electrons in an atom. Thus not all of the solutions $\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t)$ to the Schrödinger equation (2.17) can be physically permissible. Consider the case where the system contains only one species of identical particles, for example electrons. The Hamilton operator in Eq. (2.17) is invariant under all permutations of the particle labels ν. In addition, all probability amplitudes $\langle\psi_1|\psi_2\rangle$ must reflect this invariance. They must form a representation space of all permutations. Let T_{ij} be an operator which interchanges the variables $\mathbf{x}_i$ and $\mathbf{x}_j$.

$$T_{ij}\psi(\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots, \mathbf{x}_n; t) \equiv \psi(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_i, \dots, \mathbf{x}_n; t). \tag{2.20}$$

It is called a *transposition*. The invariance may then be expressed as $\langle T_{ij}\psi_1|T_{ij}\psi_2\rangle = \langle\psi_1|\psi_2\rangle$, implying that the wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$ can change at most by a phase:

$$T_{ij}\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = e^{i\alpha_{ij}}\psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \tag{2.21}$$

But from the definition (2.20) we see that T_{ij} satisfies

$$T_{ij}^2 = 1. \tag{2.22}$$

Thus $e^{i\alpha_{ij}}$ can only have the values $+1$ or -1. Moreover, due to the identity of all particles, the sign must be the same for any pair ij. As a consequence, the wave functions of n identical particles are either all completely symmetric or completely antisymmetric. In nature both signs can occur. Particles with symmetric wave functions are called *bosons*, the others *fermions*. Examples for bosons are photons, mesons, α-particles or any nuclei with an even atomic number, examples for fermions are electrons, neutrinos, muons, protons, neutrons, or any nuclei with an odd atomic number.

In two-dimensional multi-electron systems in very strong magnetic fields an interesting new situation has been discovered. These systems have wave functions which look like those of free quasiparticles on which transpositions T_{ij} yield a phase factor $e^{i\alpha_{ij}}$ which is not equal to ± 1: These quasiparticles are neither bosons nor fermions, and have therefore been called *anyons*. Their existence in two dimension is made possible by imagining each particle to introduce a singularity in the plane which makes the plane multisheeted. A second particle moving by 360^0 around this singularity does not arrive at the initial point but at a point lying in a second sheet below the initial point. For this reason, the equation (2.22) need no longer be fulfilled.

The symmetry properties of the wave functions considerably increase the work in dealing with the Schrödinger equation. Let us illustrate this by looking at the simplest nontrivial case in which the particles have only a common time-independent external potential $V_1(\mathbf{x}_\nu)$ but are otherwise noninteracting, i.e., their time-independent Schrödinger equation (2.19) reads

$$\sum_\nu \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}_\nu}^2 + V_1(\mathbf{x}_\nu) \right] \psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n) = E \psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n). \tag{2.23}$$

It can be solved by the factorizing ansatz in terms of single-particle states $\psi_{E_{\alpha_\nu}}$ of energy E_{α_ν},

$$\psi_E(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \prod_{\nu=1}^{n} \psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu), \tag{2.24}$$

with the total energy being the sum of the individual energies:

$$E = \sum_{\nu=1}^{n} E_{\alpha_\nu}. \tag{2.25}$$

The single-particle states $\psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu)$ are the solutions of the one-particle Schrödinger equation

$$\left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}}^2 + V_1(\mathbf{x}) \right] \psi_{E_\alpha}(\mathbf{x}) = E_\alpha \psi_{E_\alpha}(\mathbf{x}). \tag{2.26}$$

If the wave functions $\psi_{E_\alpha}(\mathbf{x})$ form a complete set of states, they satisfy the one-particle completeness relation

$$\sum_\alpha \psi_{E_\alpha}(\mathbf{x}) \psi_{E_\alpha}^*(\mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.27}$$

The sum over the labels α may, of course, involve an integral over a continuous part of the spectrum. It is trivial to verify that the set of all products (2.24) is complete in the space of n-particle wave functions:

$$\sum_{\alpha_1, \ldots, \alpha_n} \psi_{E_{\alpha_1}}(\mathbf{x}_1) \cdots \psi_{E_{\alpha_n}}(\mathbf{x}_n) \, \psi_{E_{\alpha_n}}^*(\mathbf{x}_n') \cdots \psi_{E_{\alpha_1}}^*(\mathbf{x}_1')$$
$$= \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}_1') \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}_n'). \tag{2.28}$$

For identical particles, this Hilbert space is greatly reduced. In the case of bosons, only the fully symmetrized products

$$\psi^S_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n) = \mathcal{N}^S_{\{E_\alpha\}}\frac{1}{n!}\sum_P\prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu) \tag{2.29}$$

correspond to physical energy eigenstates. The sum runs over $n!$ permutations of the indices $\nu = 1,\dots,n$, the permuted indices being denoted by $p(\nu)$.

Note that $\psi^S_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n)$ no longer depends on the order of the labels on the energies $E_{\alpha_1},\dots,E_{\alpha_n}$. This is a manifestation of the indistinguishability of the particles in the corresponding one-particle states. We have indicated this by the curly brackets notation $\psi^S_{\{E_\alpha\}}$. Also the normalization factor is independent of the order and has been denoted by $\mathcal{N}^S_{\{E_\alpha\}}$.

For fermions, the wave functions are

$$\psi^A_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n) = \mathcal{N}^A_{\{E_\alpha\}}\frac{1}{n!}\sum_P\epsilon_P\prod_{\nu=1}^n \psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu), \tag{2.30}$$

where $\epsilon_P = \pm 1$ for even or odd permutations, respectively.

Instead of the indices on the labels α_ν, we may just as well symmetrize or antisymmetrize those on the position variables:

$$\psi^{S,A}_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n) = \mathcal{N}^{S,A}_{\{E_\alpha\}}\frac{1}{n!}\sum_P\left\{\begin{array}{c}1\\ \epsilon_P\end{array}\right\}\prod_{\nu=1}^n \psi_{E_{\alpha_\nu}}(\mathbf{x}_{p(\nu)}). \tag{2.31}$$

See Appendix 2A for more details.

The completely antisymmetrized products (2.30) can also be written in the form of a determinant introduced first by Slater:

$$\psi^A_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n) = \mathcal{N}^A_{\{E_\alpha\}}\frac{1}{n!}\left|\begin{array}{cccc}\psi_{E_{\alpha_1}}(\mathbf{x}_1) & \psi_{E_{\alpha_1}}(\mathbf{x}_2) & \dots & \psi_{E_{\alpha_1}}(\mathbf{x}_n)\\ \vdots & \vdots & & \vdots\\ \psi_{E_{\alpha_n}}(\mathbf{x}_1) & \psi_{E_{\alpha_n}}(\mathbf{x}_2) & \dots & \psi_{E_{\alpha_n}}(\mathbf{x}_n)\end{array}\right|. \tag{2.32}$$

To determine the normalization factors in (2.29)–(2.32), we calculate the integral

$$\begin{aligned}\int d^3x_1\cdots d^3x_n\,&\psi^{S\,*}_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n)\psi^S_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n)\\ &= \mathcal{N}^{S\;2}_{\{E_\alpha\}}\frac{1}{n!^2}\sum_{P,Q}\prod_{\nu=1}^n\int d^3x_\nu\psi^*_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu)\psi_{E_{\alpha_{q(\nu)}}}(\mathbf{x}_\nu).\end{aligned} \tag{2.33}$$

Due to the group property of permutations, the double-sum contains $n!$ identical terms with $P = Q$ and can be rewritten as

$$\begin{aligned}\int d^3x_1\cdots d^3x_n\,&\psi^{S\,*}_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n)\psi^S_{\{E_\alpha\}}(\mathbf{x}_1,\dots,\mathbf{x}_n)\\ &= \mathcal{N}^{S\;2}_{\{E_\alpha\}}\frac{1}{n!}\sum_{P}\prod_{\nu=1}^n\int d^3x_\nu\psi^*_{E_{\alpha_\nu}}(\mathbf{x}_\nu)\psi_{E_{\alpha_{p(\nu)}}}(\mathbf{x}_\nu).\end{aligned} \tag{2.34}$$

If all single-particle states $\psi_{E_{\alpha_\nu}}(\mathbf{x}_\nu)$ are different from each other, then only the identity permutation $P = 1$ with $p(\nu) = \nu$ survives, and (2.34) results in

$$ {\mathcal{N}^{S}_{\{E_\alpha\}}}^{2} = n!. \tag{2.35}$$

Suppose now that two of the single-particle wave functions $\psi_{E_{\alpha_\nu}}$, say $\psi_{E_{\alpha_1}}$ and $\psi_{E_{\alpha_2}}$, coincide, while all others are different from these and each other. Then only two permutations survive in (2.34): those with $p(\nu) = \nu$, and those in which P is a transposition T_{ij}, an exchange of two elements (see Appendix 2A). The right-hand side of (2.35) is then reduced by a factor 2:

$$ {\mathcal{N}^{S}_{\{E_\alpha\}}}^{2} = \frac{n!}{2}. \tag{2.36}$$

Extending this consideration to n_1 identical states $\psi_{E_{\alpha_1}}, \dots, \psi_{E_{\alpha_{n_1}}}$, all $n_1!$ permutations among these give equal contributions to the normalization integral (2.34) and results in

$$ {\mathcal{N}^{S}_{\{E_\alpha\}}}^{2} = \frac{n!}{n_1!}. \tag{2.37}$$

Finally, it is easy to see that if there are groups of $n_1, n_2, \dots\ n_k$ identical states, the normalization factor is

$$ {\mathcal{N}^{S}_{\{E_\alpha\}}}^{2} = \frac{n!}{n_1! n_2! \cdots n_k!}. \tag{2.38}$$

For the antisymmetric states of fermion systems, the situation is much simpler. Here, no two states can be identical as is obvious from the Slater determinant (2.32). Similar considerations as in (2.33), (2.34) for the wave functions (2.30) lead to

$$ {\mathcal{N}^{A}_{\{E_\alpha\}}}^{2} = n!. \tag{2.39}$$

The projection into the symmetric and antisymmetric subspaces has the following effect upon the completeness relation (2.28). Multiplying it by the symmetrization or antisymmetrization operators

$$ \hat{P}^{S,A} = \frac{1}{n!} \sum_{P} \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\} \tag{2.40}$$

which may be applied upon the particle positions $\mathbf{x}_1, \dots, \mathbf{x}_n$ as in (2.31), we calculate

$$ \sum_{\alpha_1,\dots,\alpha_n} \left[\mathcal{N}^{S,A}_{\{E_\alpha\}}\right]^2 \psi^{S,A}_{\{E_\alpha\}}(\mathbf{x}_1, \dots, \mathbf{x}_n) \psi^{S,A\,*}_{\{E_\alpha\}}(\mathbf{x}'_1, \dots, \mathbf{x}'_n) = \delta^{(3)S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n), \tag{2.41}$$

where the symmetrized or antisymmetrized δ-function is defined by

$$ \delta^{(3)S,A}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n) \equiv \frac{1}{n!} \sum_{P} \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\} \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_{p(1)}) \cdots \delta^{(3)}(\mathbf{x}_n - \mathbf{x}'_{p(n)}). \tag{2.42}$$

Since the left-hand side of (2.41) is independent of the order of $E_{\alpha_1}, \ldots, E_{\alpha_n}$, we may sum only over a certain order among the labels

$$\sum_{\alpha_1,\ldots,\alpha_n} \longrightarrow n! \sum_{\alpha_1>\ldots>\alpha_n} . \tag{2.43}$$

If there are degeneracy labels in addition to the energy, these have to be ordered in the same way.

For antisymmetric states, the labels $\alpha_1, \ldots, \alpha_n$ are necessarily different from each other. Inserting (2.39) and (2.43) into (2.42), this gives directly

$$\sum_{\alpha_1>\ldots>\alpha_n} \psi^A_{\{E_\alpha\}}(\mathbf{x}_1,\ldots,\mathbf{x}_n)\psi^{A\,*}_{\{E_\alpha\}}(\mathbf{x}'_1,\ldots,\mathbf{x}'_n) = \delta^{(3)A}(\mathbf{x}_1,\ldots,\mathbf{x}_n;\mathbf{x}'_1,\ldots,\mathbf{x}'_n). \tag{2.44}$$

For the symmetric case we can order the different groups of identical states and denote their common labels by $\alpha_{n_1}, \alpha_{n_2}, \ldots, \alpha_{n_k}$, with the numbers n_ν indicating how often the corresponding label α is present. Obviously, there are $n!/n_1!n_2!\cdots n_k!$ permutations in the completeness sum (2.41) for each set of labels $\alpha_{n_1} > \alpha_{n_2} > \ldots > \alpha_{n_k}$, the divisions by $n_\nu!$ coming from the permutations *within* each group of $n_1, \ldots, n_k$ identical states. This combinatorial factor cancels precisely the normalization factor (2.38), so that the completeness relation for symmetric n-particle states reads

$$\begin{aligned}\sum_{n_1,\ldots,n_k}\ \sum_{\alpha_{n_1}>\ldots>\alpha_{n_k}} &\psi^S_{\{E_\alpha\}}(\mathbf{x}_1,\ldots,\mathbf{x}_n)\psi^{S\,*}_{\{E_\alpha\}}(\mathbf{x}'_1,\ldots,\mathbf{x}'_n)\\ &= \delta^{(3)S}(\mathbf{x}_1,\ldots,\mathbf{x}_n;\mathbf{x}'_1,\ldots,\mathbf{x}'_n).\end{aligned} \tag{2.45}$$

The first sum runs over the different breakups of the total number n of states into identical groups so that $n = n_1 + \ldots + n_k$.

It is useful to describe the symmetrization or antisymmetrization procedure directly in terms of Dirac's bra and ket formalism. The n-particle states are direct products of single-particle states multiplied by the operator $\hat{P}^{S,A}$ and can be written as:

$$|\psi^{S,A}\rangle = \hat{P}^{S,A}|E_{\alpha_1}\rangle\cdots|E_{\alpha_n}\rangle = \mathcal{N}^{S,A}\frac{1}{n!}\sum_P \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\} |E_{\alpha_{p(1)}}\rangle\cdots|E_{\alpha_{p(n)}}\rangle. \tag{2.46}$$

The wave functions (2.29) and (2.30) consist of scalar products of these states with the localized boson states $|\mathbf{x}_1,\ldots,\mathbf{x}_n\rangle$ which may be written in factorized form as

$$|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n\rangle = |\mathbf{x}_1\rangle \otimes |\mathbf{x}_2\rangle \otimes \ldots \otimes |\mathbf{x}_n\rangle. \tag{2.47}$$

In this state, particle one sits at $\mathbf{x}_1$, particle two at $\mathbf{x}_2$, ..., etc. The symmetrization process wipes out the distinction between the particles 1 to n.

Let us adapt the symbolic completeness relation to the symmetry of the wave functions. The general relation

$$\int d^3x_1\cdots d^3x_n\, |\mathbf{x}_1\rangle\langle\mathbf{x}_1| \otimes \ldots \otimes |\mathbf{x}_n\rangle\langle\mathbf{x}_n| = 1 \tag{2.48}$$

covers *all* square integrable wave functions in the product space. As far as the physical Hilbert space is concerned, it can be restricted as follows

$$\int d^3x_1 \cdots d^3x_n \, |\mathbf{x}_1,\ldots,\mathbf{x}_n\rangle^{S,A} \; {}^{S,A}\langle \mathbf{x}_1,\ldots,\mathbf{x}_n| = \hat{P}^{S,A}, \tag{2.49}$$

where

$$|\mathbf{x}_1,\ldots,\mathbf{x}_n\rangle^{S,A} \;=\; \frac{1}{n!}\sum_P \left\{ \begin{array}{c} 1 \\ \epsilon_P \end{array} \right\} |\mathbf{x}_{p(1)},\ldots,\mathbf{x}_{p(n)}\rangle. \tag{2.50}$$

The states are orthonormal in the sense

$${}^{S,A}\langle \mathbf{x}_1,\ldots,\mathbf{x}_n|\mathbf{x}_1',\ldots,\mathbf{x}_n'\rangle^{S,A} = \delta^{(3)S,A}(\mathbf{x}_1,\ldots,\mathbf{x}_n;\mathbf{x}_1',\ldots,\mathbf{x}_n'). \tag{2.51}$$

This basis will play an essential role for the introduction of quantum fields.

While the formalism presented so far is applicable to any number of particles, practical calculations usually present a tremendous task. The number of particles is often so large, of the order 10^{23}, that no existing computer could even list the wave functions. On the other hand, macroscopic many-body systems containing such a large number of microscopic particles make up our normal environment and our experience teaches us that many global phenomena can be predicted quite reliably. They should therefore also be calculable in simple terms. For example, for most purposes a crystal follows the laws of a rigid body and nothing in this laws records the immense number of degrees of freedom inherent in a microscopic description. If the solid is exited, there are sound waves in which all the many atoms in the lattice vibrate around their equilibrium positions. Their description requires only a few bulk parameters such as elastic constants and mass density. Phenomena of this type are called *collective phenomena.*

To describe such phenomena, an economic way has to be found which does not require the solution of the Schrödinger differential equation with $3n \sim 10^{23}$ coordinates. We shall see later that field theory provides us with an elegant and economical access to such phenomena. After a suitable choice of field variables, simple mean-field approximations will often give a rough explanation of many collective phenomena. In the subsequent sections we shall demonstrate how the Schrödinger theory of any number of particles can be transformed into the quantum field theory of a single field.

There is a further motivation at a more fundamental level for introducing fields. They offer a natural way of accounting for the symmetry properties of the wave functions, as we shall now see.

2.3 Creation and Annihilation Operators for Bosons

When dealing with n-particle Schrödinger equations, the imposition of symmetry upon the Schrödinger wave functions $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t)$ seems to be a rather artificial procedure. There exists an alternative formulation of the quantum mechanics of

n particles in which the Hilbert space *automatically* carries the correct symmetry. This formulation may therefore be viewed as a more "natural" description of such quantum systems. The basic mathematical structure which will serve this purpose is first encountered in a particular quantum mechanical description of harmonic oscillators which we now recall. It is well-known that the Hamilton operator of an oscillator of unit mass

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{\omega^2}{2}\hat{q}^2 \tag{2.52}$$

can be rewritten in the form

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{2.53}$$

where

$$\hat{a}^\dagger = \frac{\sqrt{\omega}\hat{q} - i\hat{p}/\sqrt{\omega}}{\sqrt{2\hbar}}, \qquad \hat{a} = \frac{\sqrt{\omega}\hat{q} + i\hat{p}/\sqrt{\omega}}{\sqrt{2\hbar}} \tag{2.54}$$

are the so-called *raising* and *lowering* operators. The canonical quantization rules

$$\begin{aligned} [\hat{p}, \hat{p}] &= [\hat{x}, \hat{x}] = 0, \\ [\hat{p}, \hat{x}] &= -i\hbar \end{aligned} \tag{2.55}$$

imply that $\hat{a}, \hat{a}^\dagger$ satisfy

$$\begin{aligned} [\hat{a}, \hat{a}] &= [\hat{a}^\dagger, \hat{a}^\dagger] = 0, \\ [\hat{a}, \hat{a}^\dagger] &= 1. \end{aligned} \tag{2.56}$$

The energy spectrum of the oscillator follows directly from these commutation rules. We introduce the *number operator*

$$\hat{N} = \hat{a}^\dagger\hat{a} \tag{2.57}$$

which satisfies the equations

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger, \tag{2.58}$$

$$[\hat{N}, \hat{a}] = -\hat{a}. \tag{2.59}$$

These imply that $\hat{a}^\dagger$ and $\hat{a}$ increase and decrease eigenvalues of the number operator $\hat{N}$ by one unit, respectively. Indeed, if $|\nu\rangle$ is an eigenstate with eigenvalue ν,

$$\hat{N}|\nu\rangle = \nu|\nu\rangle, \tag{2.60}$$

we see that

$$\begin{aligned} \hat{N}\hat{a}^\dagger|\nu\rangle &= (\hat{a}^\dagger\hat{N} + \hat{a}^\dagger)|\nu\rangle = (\nu + 1)\hat{a}^\dagger|\nu\rangle, \\ \hat{N}\hat{a}|\nu\rangle &= (\hat{a}\hat{N} - \hat{a})|\nu\rangle = (\nu - 1)\hat{a}|\nu\rangle. \end{aligned} \tag{2.62}$$

Moreover, the eigenvalues ν must all be integer numbers n larger or equal to zero. To see this we observe that $\hat{a}^\dagger\hat{a}$ is a positive operator aince for everay state $|\psi\rangle$ in the Hilbert space

$$\langle\psi|\hat{a}^\dagger\hat{a}|\psi\rangle = \|\hat{a}^\dagger|\psi\rangle\|^2 \geq 0. \tag{2.63}$$

Hence there must be a state, usually denoted by $|0\rangle$, whose energy cannot be lowered by one more application of $\hat{a}$, so that it must satisfy

$$\hat{a}|0\rangle = 0. \tag{2.64}$$

But then the operator $\hat{N}$ applied to $|0\rangle$ must be zero. Applying the raising operator $\hat{a}^\dagger$ any number of times, the eigenvalues ν of $\hat{N}$ will cover all integer numbers $\nu = n$ with $n = 0, 1, 2, 3, \ldots$. The corresponding states are denoted by $|n\rangle$:

$$\hat{N}|n\rangle = n|n\rangle, \quad n = 0, 1, 2, 3, \ldots . \tag{2.65}$$

Explicitly, these states are given by

$$|n\rangle = \mathcal{N}_n(\hat{a}^\dagger)^n|0\rangle, \tag{2.66}$$

with some normalization factor $\mathcal{N}_n$ which can be calculated using the commutation rules (2.56), yielding

$$\mathcal{N}_n = \frac{1}{\sqrt{n!}}. \tag{2.67}$$

By considering the commutation rules (2.56) between different states $|n\rangle$ and inserting intermediate states, we derive the matrix elements of the operators $\hat{a}, \hat{a}^\dagger$:

$$\langle n'|\hat{a}|n\rangle = \sqrt{n}\,\delta_{n',n-1}, \tag{2.68}$$

$$\langle n'|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,\delta_{n',n+1}. \tag{2.69}$$

In this way, all properties of the harmonic oscillator are recovered by purely algebraic manipulations using (2.56) and the condition (2.64) defining the ground state.

This mathematical structure can be used to describe the complete set of symmetric localized states (2.29). All we need to do is reinterprete the eigenvalue n of the operator $\hat{N}$, which in the case of the oscillator is the quantum number of the single-particle state, as the *number of particles contained in an n-particle state.* The operators $\hat{a}^\dagger$ and $\hat{a}$ which raise and lower n are renamed *creation* and *annihilation operators* which add or take away a single particle in the state $|n\rangle$. The ground state $|0\rangle$ contains no particle. It constitutes the vacuum state of the n-body system. In the states (2.29) there are n particles at places $\mathbf{x}_1, \ldots, \mathbf{x}_n$. We therefore introduce the spatial degree of freedom by giving $\hat{a}^\dagger, \hat{a}$ a spatial label and defining the operators

$$\hat{a}^\dagger_{\mathbf{x}}, \hat{a}_{\mathbf{x}},$$

which permit the creation and annihilation of a particle localized at the point $\mathbf{x}$.[1]

---

[1] The label $\mathbf{x}$ in configuration space of the particles bears no relation to the operator $\hat{q}$ in the Hamiltonian (2.52) which is an operator in field space, as we shall understand better in Section 2.8.

The operators at different locations are taken to be independent, i.e., they commute as

$$[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}] = [\hat{a}^\dagger_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}] = 0, \tag{2.70}$$

$$[\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}] = 0, \quad \mathbf{x} \neq \mathbf{x}'. \tag{2.71}$$

The commutation rule between $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}'}$ for coinciding space variables $\mathbf{x}$ and $\mathbf{x}'$ are specified with the help of a Dirac δ-function as follows:

$$[\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}] = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{2.72}$$

We shall refer to these $\mathbf{x}$-dependent commutation rules as the *local oscillator algebra.*

The δ-function singularity in (2.72) is dictated by the fact that we want to preserve the raising and lowering commutation rules (2.58) and (2.59) for the particle number at each point $\mathbf{x}$, i.e., we want that

$$[\hat{N}, \hat{a}^\dagger_{\mathbf{x}}] = \hat{a}^\dagger_{\mathbf{x}}, \tag{2.73}$$

$$[\hat{N}, \hat{a}_{\mathbf{x}}] = -\hat{a}_{\mathbf{x}}. \tag{2.74}$$

The total particle number operator is then given by the integral

$$\hat{N} = \int d^3x \, \hat{a}^\dagger_{\mathbf{x}} \hat{a}_{\mathbf{x}}. \tag{2.75}$$

Due to (2.71), all parts in the integral (2.75) with $\mathbf{x}'$ different from the $\mathbf{x}$ in (2.73) and (2.74) do not contribute. If the integral is to give the right-hand sides in (2.73) and (2.74), the commutator has to be equal to the δ-function.

The use of the δ-functions is of course completely analogous to that in Subsection 1.2 [recall the limiting process in Eqs. (1.82) and (1.85)]. In fact, we could introduce usual creation and annihilation operators with ordinary unit commutation rules at each point by discretizing the space into a fine point-lattice of a small lattice spacing ϵ, with discrete lattice points at

$$\mathbf{x}_{\mathbf{n}} = (n_1, n_2, n_3)\epsilon, \qquad n_\nu = 0, \pm 1, \pm 2, \dots \,. \tag{2.76}$$

For the creation or annihilation of a particle in the small cubic box around $\mathbf{x}_{\mathbf{n}}$ we use the operators $\hat{a}^\dagger_{\mathbf{n}}$ or $\hat{a}_{\mathbf{n}}$, which satisfy the discrete commutation rules

$$[\hat{a}_{\mathbf{n}}, \hat{a}_{\mathbf{n}'}] = [\hat{a}^\dagger_{\mathbf{n}}, \hat{a}^\dagger_{\mathbf{n}'}] = 0, \tag{2.77}$$

$$[\hat{a}_{\mathbf{n}}, \hat{a}^\dagger_{\mathbf{n}'}] = \delta^{(3)}_{\mathbf{n}\mathbf{n}'}, \tag{2.78}$$

and the total particle number operator is

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}^\dagger_{\mathbf{n}} \hat{a}_{\mathbf{n}}. \tag{2.79}$$

Obviously, we may identify $\hat{a}_{\mathbf{n}}$ with the discrete subset of the continuous set of operators $\hat{a}_{\mathbf{x}}$ as follows:

$$\hat{a}_{\mathbf{n}} = \sqrt{\epsilon^3} \, \hat{a}_{\mathbf{x}} \Big|_{\mathbf{x} \equiv \mathbf{x}_{\mathbf{n}}} . \tag{2.80}$$

Then the discrete and continuous formulations of the particle number operator are related by

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}^\dagger_{\mathbf{n}} \hat{a}_{\mathbf{n}} \equiv \epsilon^3 \sum_{\mathbf{x}_{\mathbf{n}}} \hat{a}^\dagger_{\mathbf{x}_{\mathbf{n}}} \hat{a}_{\mathbf{x}_{\mathbf{n}}} \xrightarrow[\epsilon\to 0]{} \int d^3x \, \hat{a}^\dagger_{\mathbf{x}} \hat{a}_{\mathbf{x}}. \tag{2.81}$$

In the same limit, the commutator

$$\frac{1}{\epsilon^3} [\hat{a}_{\mathbf{n}}, \hat{a}^\dagger{}_{\mathbf{n}'}] \equiv [\hat{a}_{\mathbf{x}_{\mathbf{n}}}, \hat{a}^\dagger_{\mathbf{x}_{\mathbf{n}'}}] = \frac{1}{\epsilon^3} \delta^{(3)}_{\mathbf{n}\mathbf{n}'} \tag{2.82}$$

tends to $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$, as can be seen in the same way as in Eq. (1.85).

We are now ready to define the vacuum state of the many-particle system. It is given by the unique state $|0\rangle$ of the local oscillator algebra (2.70) and (2.71), which contains no particle at *all* places $\mathbf{x}$, thus satisfying

$$\hat{a}_{\mathbf{x}}|0\rangle \equiv 0, \qquad \langle 0|\hat{a}^\dagger_{\mathbf{x}} \equiv 0. \tag{2.83}$$

It will always be normalized to unity:

$$\langle 0|0\rangle = 1. \tag{2.84}$$

We can now convince ourselves that the fully symmetrized Hilbert space of all localized states of n particles may be identified with the states created by repeated application of the local creation operators $\hat{a}^\dagger_{\mathbf{x}}$:

$$|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle^S \equiv \frac{1}{\sqrt{n!}} \hat{a}^\dagger_{\mathbf{x}_1} \cdots \hat{a}^\dagger_{\mathbf{x}_n} |0\rangle. \tag{2.85}$$

The so generated Hilbert space will be referred to as the *second-quantized Hilbert space* for reasons to be seen below. It decomposes into a direct sum of n-particle sectors. The symmetry of these states in the position variables is obvious due to the commutativity (2.70) of all $\hat{a}^\dagger_{\mathbf{x}_\nu}, \hat{a}^\dagger_{\mathbf{x}_\mu}$ among each other.

Let us check that the generalized orthonormality relation is indeed fulfilled by these states. Using the local commutation rules (2.70), (2.71), and the definition of the vacuum state (2.83), we calculate for one particle

$$\begin{aligned} {}^S\langle \mathbf{x}|\mathbf{x}'\rangle^S &= \langle 0|\hat{a}_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}'}|0\rangle \\ &= \langle 0|\delta^{(3)}(\mathbf{x}-\mathbf{x}') + \hat{a}^\dagger_{\mathbf{x}'} \hat{a}_{\mathbf{x}}|0\rangle \\ &= \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \end{aligned} \tag{2.86}$$

For two particles we find

$$\begin{aligned} {}^S\langle \mathbf{x}_1, \mathbf{x}_2|\mathbf{x}'_1, \mathbf{x}'_2\rangle^S &= \frac{1}{2!} \langle 0|\hat{a}_{\mathbf{x}_2} \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}^\dagger_{\mathbf{x}'_2}|0\rangle \\ &= \frac{1}{2!} \left[\delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \langle 0|\hat{a}_{\mathbf{x}_2} \hat{a}^\dagger_{\mathbf{x}'_2}|0\rangle + \langle 0|\hat{a}_{\mathbf{x}_2} \hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}'_2}|0\rangle \right] \\ &= \frac{1}{2!} \left[\delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_1) \delta^{(3)}(\mathbf{x}_2 - \mathbf{x}'_2) + \delta^{(3)}(\mathbf{x}_2 - \mathbf{x}'_1) \delta^{(3)}(\mathbf{x}_1 - \mathbf{x}'_2) \right] \\ &= \delta^{(3)S}(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}'_1, \mathbf{x}'_2). \end{aligned} \tag{2.87}$$

The generalization to n particles is straightforward but somewhat tedious. It is left to the reader as an exercise. Later in Section 5.12.1, rules will be derived in a different context by a procedure due to Wick, which greatly simplify calculations of this type.

2.4 Schrödinger Equation of Noninteracting Bosons in Terms of Creation and Annihilation Operators

Expressing the localized states in terms of the local creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}, \hat{a}_{\mathbf{x}}$ does not only lead to an automatic symmetrization of the states. It also brings about an extremely simple unified form of the Schrödinger equation which does not involve the initial specification of the particle number n to be considered, as in Eq. (2.17). This will now be shown for the case of identical particles without two-body interaction $V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t)$.

In order to exhibit the unified Schrödinger equation for any number of particles let us first neglect interactions and consider only the motion of the particles in an external potential with the Schrödinger equation

$$\left\{\sum_\nu \left[-\frac{\hbar^2}{2M}\partial^2_{\mathbf{x}_\nu} + V_1(\mathbf{x}_\nu;t)\right]\right\}\psi(\mathbf{x}_1,\dots,\mathbf{x}_n;t) = i\hbar\partial_t\psi(\mathbf{x}_1,\dots,\mathbf{x}_n;t). \tag{2.88}$$

We shall now demonstrate that the $\hat{a}^\dagger, \hat{a}$ -form of this equation which is valid for any n reads

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \tag{2.89}$$

where $\hat{H}(t)$ is simply the one-particle Hamiltonian sandwiched between creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}$ and integrated over $\mathbf{x}$, i.e.,

$$\hat{H}(t) = \int d^3x \hat{a}^\dagger_{\mathbf{x}}\left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2 + V_1(\mathbf{x};t)\right]\hat{a}_{\mathbf{x}}. \tag{2.90}$$

The operator (2.90) is called the *second-quantized Hamiltonian*, the equation (2.89) the *second-quantized Schrödinger equation*, and the state $|\psi(t)\rangle$ is any n-particle state in the second-quantized Hilbert space, generated by multiple application of $\hat{a}^\dagger_{\mathbf{x}}$ upon the vacuum state $|0\rangle$, as described in the last section. The operator nature of $\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}}$ accounts automatically for the many-body nature of Eq. (2.89).

This statement is proved by multiplying Eq. (2.89) from the left with

$$^S\langle\mathbf{x}_1,\dots,\mathbf{x}_n| = \frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},$$

giving

$$\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}\hat{H}(t)|\psi(t)\rangle = i\hbar\partial_t\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}|\psi(t)\rangle. \tag{2.91}$$

We now make use of the property (2.83) of the vacuum state to satisfy $\langle 0|\hat{a}^\dagger_{\mathbf{x}} = 0$. As a consequence, we may rewrite the left-hand side of (2.91) with the help of a commutator as

$$\frac{1}{\sqrt{n!}}\langle 0|[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{H}]|\psi(t)\rangle .$$

This commutator is easily calculated using the *operator chain rules*

$$\begin{aligned}[][\hat{A},\hat{B}\hat{C}] &= \hat{B}[\hat{A},\hat{C}]+[\hat{A},\hat{B}]\hat{C},\\ [\hat{A}\hat{B},\hat{C}] &= \hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B},\end{aligned} \tag{2.92}$$

from which we derive

$$\begin{aligned}[][\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^\dagger_{\mathbf{y}}\hat{a}_{\mathbf{z}}] &= [\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^\dagger_{\mathbf{y}}]\hat{a}_{\mathbf{z}}\\ &= \hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_3}\hat{a}_{\mathbf{x}_2}[\hat{a}_{\mathbf{x}_1},\hat{a}^\dagger_{\mathbf{y}}]\hat{a}_{\mathbf{z}}+[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_3}\hat{a}_{\mathbf{x}_2},\hat{a}^\dagger_{\mathbf{y}}]\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{z}}\\ &\;\vdots\\ &= \sum_\nu \delta^{(3)}(\mathbf{x}_\nu-\mathbf{y})\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{z}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}.\end{aligned} \tag{2.93}$$

Multiplying this by

$$\delta^{(3)}(\mathbf{y}-\mathbf{z})\left[-\hbar^2\partial_{\mathbf{z}}{}^2/2M+V_1(\mathbf{z};t)\right],$$

an integral over $d^3y\,d^3z$ gives, using (2.90),

$$[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{H}(t)]=\sum_\nu\left[-\frac{\hbar^2}{2M}\partial^2_{\mathbf{x}_\nu}+V_1(\mathbf{x}_\nu;t)\right]\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_\nu}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}, \tag{2.94}$$

so that, indeed,

$$\sum_\nu\left[-\frac{\hbar^2}{2M}\partial^2_{\mathbf{x}_\nu}+V_1(\mathbf{x}_\nu;t)\right]\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}|\psi(t)\rangle = i\hbar\partial_t\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}|\psi(t)\rangle, \tag{2.95}$$

which is precisely the n-body Schrödinger equation (2.88) with the wave function

$$\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t)\equiv\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}|\psi\,(t)\rangle . \tag{2.96}$$

2.5 Second Quantization and Symmetrized Product Representation

It is worth pointing out that the mathematical structure exploited in the process of second quantization is of a very general nature.

Consider a set of matrices M_i with indices α',α

$$(M_i)_{\alpha'\alpha}$$

which satisfy some matrix commutation rules, say

$$\left[M_i, M_j\right] = i f_{ijk} M_k. \tag{2.97}$$

Let us sandwich these matrices between creation and annihilation operators which satisfy

$$\begin{aligned} [\hat{a}_\alpha, \hat{a}_{\alpha'}] &= [\hat{a}^\dagger_\alpha, \hat{a}^\dagger_{\alpha'}] = 0, \\ [\hat{a}_\alpha, \hat{a}^\dagger_{\alpha'}] &= \delta_{\alpha\alpha'}, \end{aligned} \tag{2.98}$$

and form the analogs of "second-quantized operators"

$$\hat{M}_i \equiv \hat{a}^\dagger_{\alpha'} (M_i)_{\alpha'\alpha} \hat{a}_\alpha = \hat{a}^\dagger M_i \hat{a}. \tag{2.99}$$

Repeated indices imply a summation over all α. This is commonly referred to as *Einstein's summation convention*. In the last expression we have suppressed the indices α, α', for brevity. It is then easy to verify, using the *operator chain rules* (2.92), that the operators $\hat{M}_i$ satisfy the same commutation rules as the matrices M_i:

$$\begin{aligned} \left[\hat{M}_i, \hat{M}_j\right] &= \left[\hat{a}^\dagger M_i \hat{a}, \hat{a}^\dagger M_j \hat{a}\right] \\ &= \left[\hat{a}^\dagger M_i \hat{a}, \hat{a}^\dagger\right] M_j \hat{a} + \hat{a}^\dagger M_j \left[\hat{a}^\dagger M_i \hat{a}, \hat{a}\right] \\ &= \hat{a}^\dagger M_i M_j \hat{a} - \hat{a}^\dagger M_j M_i \hat{a} \\ &= \hat{a}^\dagger \left[M_i, M_j\right] \hat{a} = i f_{ijk} \hat{a}^\dagger M_k \hat{a} = i f_{ijk} \hat{M}_k. \end{aligned} \tag{2.100}$$

Thus the "second-quantized" operators $\hat{M}_i$ generate an *operator representation* of the matrices M_i. They can be sandwiched between states in the "second-quantized" Hilbert space generated by applying products of creation operators $\hat{a}^\dagger_n$ upon the vacuum state $|0\rangle$. Thereby they are mapped into an infinite-dimensional matrix representation. On each subspace spanned by the products of a fixed number of creation operators, they generate the symmetrized part of the direct product representation.

The action of the "second-quantized" operators $\hat{M}_i$ upon the large Hilbert space is very simple to calculate. The only commutation rules required are

$$\begin{aligned} \left[\hat{M}_i, \hat{a}^\dagger_\alpha\right] &= \hat{a}^\dagger_{\alpha'} (M_i)_{\alpha'\alpha}, \\ \left[\hat{a}_{\alpha'}, \hat{M}_i\right] &= (M_i)_{\alpha'\alpha} \hat{a}_\alpha. \end{aligned} \tag{2.101}$$

From this property we calculate directly the action upon "single-particle states":

$$\begin{aligned} \hat{M}_i \hat{a}^\dagger_\alpha |0\rangle &= \left[\hat{M}_i, \hat{a}^\dagger_\alpha\right] |0\rangle = \hat{a}^\dagger_{\alpha'} |0\rangle (M_i)_{\alpha'\alpha}, \\ \langle 0| \hat{a}_{\alpha'} \hat{M}_i &= \langle 0| \left[\hat{a}_{\alpha'}, \hat{M}_i\right] = (M_i)_{\alpha'\alpha} \langle 0| \hat{a}_\alpha. \end{aligned} \tag{2.102}$$

Thus the states $\hat{a}^\dagger_\alpha |0\rangle$ span an invariant subspace and are transformed into each other via the matrix $(M_i)_{\alpha'\alpha}$.

Consider now a state with two particles

$$\hat{a}^{\dagger}_{\alpha_1}\hat{a}^{\dagger}_{\alpha_2}|0\rangle. \tag{2.103}$$

Applying $\hat{M}_i$ to this state yields

$$\begin{aligned}\left[\hat{M}_i,\hat{a}^{\dagger}_{\alpha_1}\hat{a}^{\dagger}_{\alpha_2}\right] &= \left[\hat{M}_i,\hat{a}^{\dagger}_{\alpha_1}\right]\hat{a}^{\dagger}_{\alpha_2}+\hat{a}^{\dagger}_{\alpha_1}\left[\hat{M}_i,\hat{a}^{\dagger}_{\alpha_2}\right]\\ &= \hat{a}^{\dagger}_{\alpha'_1}\hat{a}^{\dagger}_{\alpha'_2}\left[(M_i)_{\alpha'_1\alpha_1}\delta_{\alpha'_2\alpha_2}+\delta_{\alpha'_1\alpha_1}(M_i)_{\alpha'_2\alpha_2}\right].\end{aligned} \tag{2.104}$$

Multiplying Eq. (2.104) by $|0\rangle$ from the right, we find the transformation law for the two-particle states $\hat{a}^{\dagger}_{\alpha_1}\hat{a}^{\dagger}_{\alpha_2}|0\rangle$. They are transformed via the representation matrices

$$(M_i)_{\alpha'_1\alpha'_2,\alpha_1\alpha_2}=(M_i)_{\alpha'_1\alpha_1}\delta_{\alpha'_2\alpha_2}+\delta_{\alpha'_1\alpha_1}(M_i)_{\alpha'_2\alpha_2}. \tag{2.105}$$

Omitting the indices we may also write the matrices as

$$M_i^{(2)}=M_i\times 1+1\times M_i, \tag{2.106}$$

which is the well-known way of forming representations of a matrix algebra in a direct product space.

Since $a^{\dagger}_{\alpha_1}$ and $a^{\dagger}_{\alpha_2}$ commute with each other, the invariant space constructed in this way contains only symmetric tensors and only the completely symmetrized part of the matrices $(M_i)_{\alpha'_1\alpha'_2,\alpha_1\alpha_2}$ can become active.

The alert reader will have realized that the same operator structure can be obtained for the *antisymmetrized* parts of the matrices $(M_i)_{\alpha'_1\alpha'_2,\alpha_1\alpha_2}$ by using creation and annihilation operators $a^{\dagger}_{\alpha_1}$ and a_{α_2} which satisfy the algebraic rules

$$\begin{aligned}\{\hat{a}_{\alpha},\hat{a}_{\alpha'}\} &= \{\hat{a}^{\dagger}_{\alpha},\hat{a}^{\dagger}_{\alpha'}\}=0,\\ \{\hat{a}_{\alpha},\hat{a}^{\dagger}_{\alpha'}\} &= \delta_{\alpha\alpha'},\end{aligned} \tag{2.107}$$

where the curly bracket denotes the *anticommutator*

$$\{A,B\}\equiv AB+BA. \tag{2.108}$$

The first two lines in (2.100) are unchanged since the operator chain rules (2.92) hold for Bose and Fermi operators. To derive the third line we must use the additional rules

$$\begin{aligned}[\hat{A},\hat{B}\hat{C}] &= \{\hat{A},\hat{B}\}\hat{C}-\hat{B}\{\hat{A},\hat{C}\},\\ [\hat{A}\hat{B},\hat{C}] &= \hat{A}\{\hat{B},\hat{C}\}-\{\hat{A},\hat{C}\}\hat{B}.\end{aligned} \tag{2.109}$$

This fermionic version of the commutation relation (2.100) will form, in Section 2.10, the basis for constructing a second-quantized representation for the n-particle wave functions and Schrödinger operators of fermions.

If M_i are chosen to be representation matrices L_i of the generators of the rotation group (to be discussed in detail in Section 3.1), the law (2.106) represents the quantum mechanical law of addition of two angular momenta:

$$L_i^{(2)} = L_i \times 1 + 1 \times L_i.$$

The generalization to any number of angular momenta is obvious.

Incidentally, any operator which satisfies the same commutation rules with $\hat{M}_i$ as $\hat{a}_\alpha$ in (2.101),

$$\begin{aligned} \left[\hat{M}_i, \hat{O}^\dagger_\alpha\right] &= \hat{O}^\dagger_{\alpha'}(M_i)_{\alpha'\alpha}, \\ \left[\hat{O}_{\alpha'}, \hat{M}_i\right] &= (M_i)_{\alpha'\alpha}\hat{O}_\alpha, \end{aligned} \tag{2.110}$$

will be referred to as a *spinor operator*. Generalizing this definition, an operator $\hat{O}_{\alpha_1\alpha_2\ldots\alpha_n}$ which commutes with $\hat{M}_i$ like a product $\hat{O}_{\alpha_1}\hat{O}_{\alpha_2}\cdots\hat{O}_{\alpha_n}$ generalizing Eq. (2.104) is called a *multispinor operator* of rank n. Another type of operators which frequently occurs in quantum mechanics and quantum field theory is a *vector operator*, which is any operator $\hat{O}_j$ which commutes with $\hat{M}_i$ in the same way as $\hat{M}_j$ itself in (2.100), i.e.,

$$\left[\hat{M}_i, \hat{O}_j\right] = i f_{ijk}\hat{O}_k. \tag{2.111}$$

Its generalization $\hat{O}_{j_1j_2\ldots j_n}$ which commutes with $\hat{M}_i$ as the product of operators $\hat{M}_{j_1}\hat{M}_{j_2}\ldots\hat{M}_{j_n}$ is called a *tensor operator* of rank n.

The many-particle version of the Schrödinger theory is obtained if we view the one-particle Schrödinger equation

$$H(-i\hbar\partial_{\mathbf{x}}, \mathbf{x})\psi(\mathbf{x}, t) = i\hbar\partial_t\psi(\mathbf{x}, t) \tag{2.112}$$

as a matrix equation in the discretized $\mathbf{x}$-space with the lattice positions $\mathbf{x} = (n_1, n_2, n_3)\epsilon$, so that $\psi(\mathbf{x}, t)$ correspond to vectors $\psi_{\mathbf{n}}(t)$. Then the differential operator $\partial_i\psi(\mathbf{x})$ becomes simply $\nabla_i\psi(\mathbf{x}) = [\psi(\mathbf{x} + \mathbf{i}\epsilon) - \psi(\mathbf{x})]/\epsilon = \left[\psi_{\mathbf{n}+\mathbf{i}} - \psi_{\mathbf{n}}\right]/\epsilon$ where $\mathbf{i}$ is the unit vector in the ith direction and ϵ the lattice spacing. The Laplacian may be viewed as the continuum limit of the matrix

$$\begin{aligned} \bar{\nabla}_i\nabla_i\psi(\mathbf{x}) &= \frac{1}{\epsilon^2}\sum_{i=1}^{3}\left[\psi(\mathbf{x} + \mathbf{i}\epsilon) - 2\psi(\mathbf{x}) + \psi(\mathbf{x} - \mathbf{i}\epsilon)\right] \\ &= \frac{1}{\epsilon^2}\sum_{i=1}^{3}\left[\psi_{\mathbf{n}+\mathbf{i}} - 2\psi_{\mathbf{n}} + \psi_{\mathbf{n}-\mathbf{i}}\right]. \end{aligned} \tag{2.113}$$

The Schrödinger equation (2.112) is then the $\epsilon \to 0$ -limit of the matrix equation

$$H_{\mathbf{n}\mathbf{n}'}\psi_{\mathbf{n}'}(t) = i\hbar\partial_t\psi_{\mathbf{n}}(t). \tag{2.114}$$

The many-particle Schrödinger equation in second quantization form reads

$$\hat{H}|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle, \tag{2.115}$$

with the Hamilton operator

$$\hat{H} = \hat{a}^\dagger_{\mathbf{n}'} H_{\mathbf{n}'\mathbf{n}} \hat{a}_{\mathbf{n}}. \tag{2.116}$$

It can be used to find the eigenstates in the symmetrized multispinor representation space spanned by

$$\hat{a}^\dagger_{\mathbf{n}_1} \dots \hat{a}^\dagger_{\mathbf{n}_N} |0\rangle. \tag{2.117}$$

Applying $\hat{H}$ to it we see that this state is multiplied from the right by a direct-product matrix

$$H \times 1 \times \dots \times 1 + 1 \times H \times \dots \times 1 + \dots 1 \times 1 \times \dots \times H. \tag{2.118}$$

Due to this very general relation, the Schrödinger energy of a many-body system without two- or higher-body interactions is the sum of the one-particle energies.

2.6 Bosons with Two-Body Interactions

We now include two-body interactions. For simplicity, we neglect the one-body potential $V_1(\mathbf{x}; t)$ which can be added at the end and search for the second-quantized form of the Schrödinger equation

$$\left[-\sum_\nu \frac{\hbar^2}{2M} \partial^2_{\mathbf{x}_\nu} + \frac{1}{2} \sum_{\mu,\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) \right] \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t) = i\hbar \partial_t \psi(\mathbf{x}_1, \dots, \mathbf{x}_n; t). \tag{2.119}$$

It is easy to see that such a two-body potential can be introduced into the second-quantized Schrödinger equation (2.89) by adding to the Hamilton operator in (2.90) the interaction term

$$\hat{H}_{\rm int}(t) = \frac{1}{2} \int d^3x d^3x' \hat{a}^\dagger_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}'} V_2(\mathbf{x} - \mathbf{x}'; t) \hat{a}_{\mathbf{x}'} \hat{a}_{\mathbf{x}}. \tag{2.120}$$

To prove this we work out the expectation value

$$\frac{1}{\sqrt{n!}} \langle 0 | \hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1} \hat{H}_{\rm int}(t) | \psi(t) \rangle = \frac{1}{\sqrt{n!}} \langle 0 | [\hat{a}_{\mathbf{x}_n} \dots \hat{a}_{\mathbf{x}_1}, \hat{H}_{\rm int}(t)] | \psi(t) \rangle \tag{2.121}$$

with the use of the local commutation rules (2.70), (2.72), and the vacuum property (2.83). First we generalize Eq. (2.93) to

$$\begin{aligned}
&[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_2} \hat{a}^\dagger_{\mathbf{y}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2}] \\
&\quad = [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_2} \hat{a}^\dagger_{\mathbf{y}_1}] \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} \\
&\quad = [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_2}] \hat{a}^\dagger_{\mathbf{y}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} + \hat{a}^\dagger_{\mathbf{y}_2} [\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_1}] \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} \\
&\quad = \sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_2) \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{y}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} \\
&\quad\quad + \hat{a}^\dagger_{\mathbf{y}_2} \sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_1) \hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2}.
\end{aligned} \tag{2.122}$$

The second piece does not contribute to Eq. (2.121) since $\hat{a}^\dagger_{\mathbf{y}_2}$ annihilates the vacuum on the left. For the same reason, the first piece can be written as

$$\sum_\nu \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_2)[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_1}] \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} \tag{2.123}$$

as long as it stands to the right of the vacuum. Using the commutation rule (2.93), this leads to:

$$\begin{aligned} \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{y}_2} \hat{a}^\dagger_{\mathbf{y}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} |\psi(t)\rangle &= \sum_{\mu,\nu} \delta^{(3)}(\mathbf{x}_\mu - \mathbf{y}_1) \delta^{(3)}(\mathbf{x}_\nu - \mathbf{y}_2) \\ &\times \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_{\nu+1}} \hat{a}_{\mathbf{x}_{\nu-1}} \cdots \hat{a}_{\mathbf{x}_{\mu+1}} \hat{a}_{\mathbf{x}_{\mu-1}} \ldots \hat{a}_{\mathbf{x}_1} \hat{a}_{\mathbf{z}_1} \hat{a}_{\mathbf{z}_2} |\psi(t)\rangle. \end{aligned} \tag{2.124}$$

After multiplying this relation by $V_2(\mathbf{y}_2 - \mathbf{y}_1; t) \delta^{(3)}(\mathbf{y}_1 - \mathbf{z}_1) \delta^{(3)}(\mathbf{y}_2 - \mathbf{z}_2)/2$, and integrating over $d^3y_1\, d^3y_2\, d^3z_1\, d^3z_2$, we find

$$\langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} \hat{H}_{\mathrm{int}} |\psi(t)\rangle = \frac{1}{2} \sum_{\mu,\nu} V_2(\mathbf{x}_\nu - \mathbf{x}_\mu; t) \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} |\psi\,(t)\,\rangle, \tag{2.125}$$

which is precisely the two-body interaction in the Schrödinger equation (2.119).

Adding now the one-body interactions we see that an n-body Schrödinger equation with arbitrary one- and two-body potentials can be written in the form of a single operator Schrödinger equation

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle \tag{2.126}$$

with the second-quantized Hamilton operator

$$\hat{H}(t) = \int d^3x \hat{a}^\dagger_{\mathbf{x}} \left[-\frac{\hbar^2}{2M} \partial_{\mathbf{x}}{}^2 + V_1(\mathbf{x}; t) \right] \hat{a}_{\mathbf{x}} + \frac{1}{2} \int d^3x\, d^3x'\, \hat{a}^\dagger_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}'} V_2(\mathbf{x} - \mathbf{x}'; t) \hat{a}_{\mathbf{x}'} \hat{a}_{\mathbf{x}}. \tag{2.127}$$

The second-quantized Hilbert space of the states $|\psi(t)\rangle$ is constructed by repeated multiplication of the vacuum vector $|0\rangle$ with particle creation operators $\hat{a}^\dagger_{\mathbf{x}}$. The order of the creation and annihilation operators in this Hamiltonian is such that the vacuum as a zero-particle state has zero energy:

$$\hat{H}(t)|0\rangle = 0, \qquad \langle 0|\hat{H}(t) = 0, \tag{2.128}$$

as in the original Schrödinger equation.

A Hamiltonian which is a spatial integral over a *Hamiltonian density* $\mathcal{H}(\mathbf{x})$ as

$$H = \int d^3x\, \mathcal{H}(\mathbf{x}), \tag{2.129}$$

is called a *local Hamiltonian.* In (2.127), the free part is local, but the interacting part is not. It consists of an integral over two spatial variables, thus forming a *bilocal* operator.

2.7 Quantum Field Formulation of Many-Boson Schrödinger Equations

The annihilation operator $\hat{a}_{\mathbf{x}}$ can now be used to define a time-dependent quantum field $\hat{\psi}(\mathbf{x},t)$ as being the Heisenberg picture of the operator $\hat{a}_{\mathbf{x}}$ (which itself is also referred to as the Schrödinger picture of the annihilation operator). According to Eqs. (1.245), the Heisenberg operator associated with $\hat{a}_{\mathbf{x}}$ is

$$a_{\mathbf{x}\,\mathrm{H}}(t) \equiv [\hat{U}(t,t_a)]^{-1}\hat{a}_{\mathbf{x}}\hat{U}(t,t_a). \tag{2.130}$$

Thus we define

$$\hat{\psi}(\mathbf{x},t) \equiv a_{\mathbf{x}\,\mathrm{H}}(t). \tag{2.131}$$

Choosing the time variable $t_a = 0$, the quantum field $\hat{\psi}(\mathbf{x},t)$ coincides with $\hat{a}_{\mathbf{x}}$ at $t = 0$:

$$\hat{\psi}(\mathbf{x},0) \equiv \hat{a}_{\mathbf{x}}. \tag{2.132}$$

The time dependence of $\hat{\psi}(\mathbf{x},t)$ is ruled by Heisenberg's equation of motion (1.241):

$$\partial_t\hat{\psi}(\mathbf{x},t) = \frac{i}{\hbar}[\hat{H}_H(t),\hat{\psi}(\mathbf{x},t)]. \tag{2.133}$$

For simplicity, we shall at first assume the potentials to have no explicit time dependence, an assumption to be removed later. Then Eq. (2.133) is solved by

$$\hat{\psi}(\mathbf{x},t) = e^{i\hat{H}t/\hbar}\hat{\psi}(\mathbf{x},0)e^{-i\hat{H}t/\hbar} = e^{i\hat{H}t/\hbar}\hat{a}_{\mathbf{x}}e^{-i\hat{H}t/\hbar}. \tag{2.134}$$

The hermitian conjugate of this determines the time dependence of the Hesienberg picture of the creation operator:

$$\hat{\psi}^\dagger(\mathbf{x},t) = e^{i\hat{H}t/\hbar}\hat{\psi}^\dagger(\mathbf{x},0)e^{-i\hat{H}t/\hbar} = e^{i\hat{H}t/\hbar}\hat{a}^\dagger_{\mathbf{x}}e^{-i\hat{H}t/\hbar}. \tag{2.135}$$

At each given time t, the field $\hat{\psi}(\mathbf{x},t)$ fulfills the same commutation rules (2.70) and (2.71) as $\hat{a}_{\mathbf{x}}$:

$$\begin{aligned}
[\hat{\psi}(\mathbf{x},t),\hat{\psi}(\mathbf{x}',t)] &= 0,\\
[\hat{\psi}^\dagger(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)] &= 0,\\
[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)] &= \delta^{(3)}(\mathbf{x}-\mathbf{x}').
\end{aligned} \tag{2.136}$$

Consider now the Hamilton operator (2.127) in the Heisenberg representation. Under the assumption of no explicit time dependence in the potentials we may simply multiply it by $e^{i\hat{H}t/\hbar}$ and $e^{-i\hat{H}t/\hbar}$ from the left and right, respectively, and see that

$$\begin{aligned}
\hat{H}_H(t) &= \int d^3x\,\hat{\psi}^\dagger(\mathbf{x},t)\left[-\frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2+V_1(\mathbf{x})\right]\hat{\psi}(\mathbf{x},t)\\
&\quad+\frac{1}{2}\int d^3x d^3x'\,\hat{\psi}^\dagger(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t)V_2(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x}',t)\hat{\psi}(\mathbf{x},t).
\end{aligned} \tag{2.137}$$

Since $\hat{H}$ commutes with itself, the operator $\hat{H}_H(t)$ is time independent, so that

$$\hat{H}_H(t) \equiv \hat{H}. \tag{2.138}$$

The important point about the expression (2.137) for $\hat{H}$ is now that since it contains the time-dependent fields $\hat{\psi}(\mathbf{x},t)$, it can be viewed as the Hamilton operator of a canonically quantized Heisenberg field theory in analogy with the Hamiltonian $\hat{H} \equiv H(\hat{p}_H(t), \hat{x}_H(t), t)$ in (1.239). Instead of $p_H(t)$ and $q_H(t)$ we are dealing here with generalized coordinates and their canonically conjugate momenta of the field system. They consist of the hermitian and anti-hermiation parts of the field, $\hat{\psi}_R(\mathbf{x},t)$ and $\hat{\psi}_I(\mathbf{x},t)$, defined by

$$\hat{\psi}_R \equiv \frac{(\hat{\psi}+\hat{\psi}^\dagger)}{\sqrt{2}}, \qquad \hat{\psi}_I \equiv \frac{(\hat{\psi}-\hat{\psi}^\dagger)}{\sqrt{2}i}. \tag{2.139}$$

They commute like

$$\begin{aligned} [\hat{\psi}_I(\mathbf{x},t), \hat{\psi}_R(\mathbf{x}',t)] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \\ [\hat{\psi}_I(\mathbf{x},t), \hat{\psi}_I(\mathbf{x}',t)] &= 0, \\ [\hat{\psi}_R(\mathbf{x},t), \hat{\psi}_R(\mathbf{x}',t)] &= 0. \end{aligned} \tag{2.140}$$

These commutation rules are structurally identical to those between the quasi-Cartesian generalized canonical coordinates $\hat{q}_{iH}(t)$ and $\hat{p}_{iH}(t)$ in Eq. (1.22).

In fact, the formalism developed there can be generalized to an infinite set of canonical variables labeled by the space points $\mathbf{x}$ rather than i, i.e., to canonical variables $p_{\mathbf{x}}(t)$ and $q_{\mathbf{x}}(t)$. Then the quantization rules (1.22) take the form

$$\begin{aligned} [\hat{p}_{\mathbf{x}}(t), \hat{q}_{\mathbf{x}'}(t)] &= -i\hbar\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \\ [\hat{p}_{\mathbf{x}}(t), \hat{p}_{\mathbf{x}'}(t)] &= 0, \\ [\hat{q}_{\mathbf{x}}(t), \hat{q}_{\mathbf{x}'}(t)] &= 0, \end{aligned} \tag{2.141}$$

which is a local version of the algebra (2.55). The replacement $i \to \mathbf{x}$ can of course be done on a lattice with a subsequent continuum limit as in Eqs. (2.76)–(2.82). When going from the index i to the continuous spatial variable $\mathbf{x}$, the Kronecker δ_{ij} turns into Dirac's $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$, and sums become integrals.

By identifying

$$\hat{p}_{\mathbf{x}}(t) \equiv \hbar\hat{\psi}_I(\mathbf{x},t), \qquad \hat{q}_{\mathbf{x}}(t) \equiv \hat{\psi}_R(\mathbf{x},t), \tag{2.142}$$

we now obtain the commutation relations (2.140). In quantum field theory it is customary to denote the canonical momentum variable $p_{\mathbf{x}}(t)$ by the symbol $\pi_{\mathbf{x}}(t)$, and write

$$\hat{p}_{\mathbf{x}}(t) = \hbar\hat{\psi}_I(\mathbf{x},t) \equiv \hat{\pi}(\mathbf{x},t). \tag{2.143}$$

Thus the many-body nature of the system may be considered as a consequence of *quantizing the fields* $q_{\mathbf{x}}(t) = \hat{\psi}_R(\mathbf{x},t)$ and $\hat{p}_{\mathbf{x}}(t) = \hbar\hat{\psi}_I(\mathbf{x},t)$ canonically via Eq. (2.141).

2.8 Canonical Formalism in Quantum Field Theory

So far, the commutation rules have been imposed upon the fields $\hat{\psi}(\mathbf{x},t)$ and $\hat{\psi}^\dagger(\mathbf{x}',t)$ by the particle nature of the n-body Schrödinger theory. It is, however, possible to *derive* these rules from a standard canonical formalism involving the fields $\psi_R(\mathbf{x},t)$ and $\psi_I(\mathbf{x},t)$ as generalized Lagrange coordinates. To see this, let us recall once more the general procedure for finding the quantization rules and the Schrödinger equation for a general Lagrangian system with an action

$$\mathcal{A} = \int dt\, L(q(t),\dot{q}(t)), \tag{2.144}$$

where the Lagrangian L is some function of the independent variables $q(t) = (q_1(t),\dots,q_N(t))$ and their velocities $\dot{q}(t) = (\dot{q}_1(t),\dots,\dot{q}_N(t))$. The conjugate momenta are defined, as usual, by the derivatives

$$p_i(t) = \frac{\partial L}{\partial \dot{q}_i(t)}. \tag{2.145}$$

The Hamiltonian is given by the Legendre transformation

$$H(p(t),q(t)) = \sum_i p_i(t)q_i(t) - L(q(t),\dot{q}(t)). \tag{2.146}$$

If $q(t)$ are Cartesioan or quasi-Cartesian coordinates, quantum physics is imposed in the Heisenberg picture by letting $p_i(t)$, $q_i(t)$ becpme operators $\hat{p}_{iH}(t)$, $\hat{q}_{iH}(t)$ satisfying the canonical equal time commutation rules

$$\begin{aligned} [\hat{p}_{iH}(t),\hat{q}_{jH}(t)] &= -iH\hbar\delta_{ij}, \\ [\hat{p}_{iH}(t),\hat{p}_{jH}(t)] &= [\hat{q}_{iH}(t),\hat{q}_{jH}(t)] = 0, \end{aligned} \tag{2.147}$$

and postulating the Heisenberg equation of motion

$$\frac{d}{dt}\hat{O}_H = \frac{i}{\hbar}[\hat{H}_H,\hat{O}_H] + \frac{\partial}{\partial t}\hat{O}_H. \tag{2.148}$$

for any observable

$$\hat{O}_H(t) \equiv O(\hat{p}_H(t),\hat{q}_H(t),t). \tag{2.149}$$

This formalism holds for any number of Cartesian or quasi-Cartesian variables. It can therefore be generalized also to a continuous set. Changing sums into integrals, and Kronecker symbols δ_{ij} into Dirac δ-functions, the Hamiltonian reads

$$H = \int d^3x\, p_{\mathbf{x}}(t)\dot{q}_{\mathbf{x}}(t) - L[q,\dot{q}], \tag{2.150}$$

where the brackets indicate that the Lagrangian is now a functional of all $q_{\mathbf{x}}, \dot{q}_{\mathbf{x}}$. The canonical commutation rules (2.147) go over into (2.141). For continuous labels

$\mathbf{x}$, the definition (2.145) of the canonical momentum must be replaced by what is called the *functional derivative*:

$$p_{\mathbf{x}}(t)=\frac{\delta L}{\delta \dot{q}_{\mathbf{x}}(t)}, \tag{2.151}$$

defined to satisfy Leibnitz' chain rule of differentiation and the following properties:

$$\frac{\delta q_{\mathbf{x}}(t)}{\delta q_{\mathbf{x}'}(t)}=\frac{\delta \dot{q}_{\mathbf{x}}(t)}{\delta \dot{q}_{\mathbf{x}'}(t)}=\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{2.152}$$

$$\frac{\delta q_{\mathbf{x}}(t)}{\delta \dot{q}_{\mathbf{x}'}(t)}=\frac{\delta \dot{q}_{\mathbf{x}}(t)}{\delta q_{\mathbf{x}'}(t)}=0. \tag{2.153}$$

These are a direct generalization of corresponding properties of the discrete set of coordinates $q_i(t)$, $\dot{q}_i(t)$, which obey

$$\frac{\partial \dot{q}_i(t)}{\partial \dot{q}_j(t)}=\frac{\partial q_i(t)}{\partial q_j(t)}=\delta_{ij}, \tag{2.154}$$

$$\frac{\partial q_i(t)}{\partial \dot{q}_j(t)}=\frac{\partial \dot{q}_i(t)}{\partial q_j(t)}=0, \tag{2.155}$$

which express the independence of the Lagrangian coordinates. By using (2.152) and (2.153) together with the chain rule of differentiation, we can calculate all functional derivatives of an arbitrary Lagrangian L with respect to $\delta q_{\mathbf{x}}(t)$ and $\delta \dot{q}_{\mathbf{x}}(t)$.

It is quite simple to find a classical Lagrangian for which one can derive, via the standard canonical formalism, the Hamiltonian (2.137) and the canonical quantization rules in the form (2.140). It is given by

$$L(t)=\int d^3x\,\psi_I(\mathbf{x},t)\hbar\partial_t\psi_R(\mathbf{x},t)-H[\psi_I,\psi_R], \tag{2.156}$$

where $H[\psi_I,\psi_R]$ denotes the classical Hamiltonian associated with the operator $H_H(t)$ in Eq. (2.137). Indeed, with the identification (2.142), we find that the canonical momentum of the field is

$$p_{\mathbf{x}}(t)\equiv\frac{\delta L}{\delta \dot{q}_{\mathbf{x}}(t)}=\frac{\delta L}{\delta\partial_t\psi_R(\mathbf{x},t)}=\hbar\psi_I(\mathbf{x},t)\equiv\pi(\mathbf{x},t), \tag{2.157}$$

and (2.141) yields precisely the canonical quantization rules (2.140). Obviously, the Legendre transformation (2.150) turns L into the correct Hamiltonian H.

We have emphasized before that the canonical quantization rules are applicable only if the field space is quasi-Cartesian.[2] For this, the dynamical metric (1.19) has to be q-independent. This condition is violated by the interaction in the Hamiltonian (2.137). There are ambiguities in ordering the field operators in this interaction. These are, however, removed by the requirement that after quantizing the field system one wants to reproduce the n-body Schrödinger equation, which requires that the zero-body state has zero energy and thus satisfied Eq. (2.128).

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[2] See Footnote 6 on page 16.

The equivalence of n-body Schrödinger theory and the above derived canonically quantized field theory requires specification of the ordering of the field operators after having imposed the canonical commutation rules upon the fields.

The classical action

$$\mathcal{A} = \int dt\, L(t) \tag{2.158}$$

with the Lagrangian (2.156) can also be rewritten, in terms of the fields $\psi(\mathbf{x}, t)$ and $\psi^*(\mathbf{x}, t)$ as

$$\mathcal{A} = \int dt d^3x\, \psi^*(\mathbf{x}, t) i\hbar\partial_t\psi(\mathbf{x}, t) - \int dt\, H[\psi^*, \psi], \tag{2.159}$$

where we have performed a partial integration with respect to the time and neglected, as usual, the boundary terms at infinity. This action corresponds to the following Lagrangian

$$L(t) = \int d^3x\, \psi^*(\mathbf{x}, t) i\hbar\partial_t\psi(\mathbf{x}, t) - H[\psi^*, \psi], \tag{2.160}$$

which is completely equivalent to (2.156).

In analogy with the definition of a local Hamiltonian we call an action $\mathcal{A}$ *local*, if it can be written as a spacetime integral over a *Lagrangian density* $\mathcal{L}$:

$$\mathcal{A} = \int dt \int d^3x\, \mathcal{L}(\mathbf{x}, t), \tag{2.161}$$

where $\mathcal{L}(\mathbf{x}, t)$ depends only on the fields $\psi(\mathbf{x}, t)$ and their first derivatives. The free part in (2.159) is obviously local, the interacting part is bilocal [recall (2.137)].

Note that the Lagrangian (2.160) is not real. This presents no problem, however, since only the action is a physically observable quantity and this is real. Writing the Lagrangian in the form (2.160) has the advantage that we may think of $\psi(\mathbf{x}, t)$ as being complex generalized coordinates

$$q_{\mathbf{x}}(t) = \psi(\mathbf{x}, t), \tag{2.162}$$

with the conjugate momentum

$$p_{\mathbf{x}}(t) = \frac{\delta L}{\delta \dot{q}_{\mathbf{x}}(t)} = i\hbar\psi^*(\mathbf{x}, t) \tag{2.163}$$

to be denoted by

$$\pi(\mathbf{x}, t) \equiv i\hbar\psi^*(\mathbf{x}, t). \tag{2.164}$$

Then the formal application of the rules (2.141) leads again directly to the commutation rules (2.136) without the prior splitting into real and imaginary parts. Because of this convenience, the Lagrangian (2.160) will be used from now on. The action will be regarded as a function of the independent variables $\psi, \partial_t\psi, \psi^*$ with ψ^* carrying no time derivative.

In this complex-field formulation, only $\psi(\mathbf{x},t)$ has a canonical momentum, not $\psi^*(\mathbf{x},t)$. This, however, is an artifact of the use of complex field variables. Later in Section 5.4.1 we shall encounter a more severe problem where the canonical momentum of a component of the real electromagnetic vector field vanishes as a consequence of gauge invariance, requiring an essential modification of the quantization procedure.

The classical Euler-Lagrange equations of motion associated with a field theoretic action (2.158) with a Lagrangian (2.156) are a direct generalization of the Euler-Lagrange equations associated with a Lagrangian $L(q_i,\dot{q})$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}=\frac{\partial L}{\partial q_i}. \tag{2.165}$$

If we extremize an action

$$\mathcal{A}=\int dt L[q_{\mathbf{x}},\dot{q}_{\mathbf{x}}] \tag{2.166}$$

in which the Lagrangian is a functional of the infinitely many generalized coordinates $q_{\mathbf{x}}(t)$, we obtain directly

$$\frac{d}{dt}\frac{\delta L}{\delta \dot{q}_{\mathbf{x}}}=\frac{\delta L}{\delta q_{\mathbf{x}}}. \tag{2.167}$$

By extremizing the action expressed in terms of the complex fields $\psi(\mathbf{x},t)$ and $\psi^*(\mathbf{x},t)$, we obtain

$$\partial_t\frac{\delta L}{\delta \dot{\psi}(\mathbf{x},t)}=\frac{\delta L}{\delta \psi(\mathbf{x},t)}, \tag{2.168}$$

$$\partial_t\frac{\delta L}{\delta \dot{\psi}^*(\mathbf{x},t)}=\frac{\delta L}{\delta \psi^*(\mathbf{x},t)}. \tag{2.169}$$

For a hermitian action, the second equation is equivalent to the first, the two being simply the complex-conjugates of each other. Because of (2.142) and (2.139), the sum of the two equations is equivalent to (2.167). But the Euler-Lagrange equations are insensitive to an extra surface term and thus to the asymmetric treatment of ψ and ψ^* in the action (2.159). Indeed, Eq. (2.169) gives

$$\left[i\hbar\partial_t+\frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2-V_1(\mathbf{x})\right]\psi(\mathbf{x},t)=\int d\mathbf{x}'\,\psi^*(\mathbf{x}',t)V_2(\mathbf{x}-\mathbf{x}';t)\psi(\mathbf{x}',t)\,\psi(\mathbf{x},t), \tag{2.170}$$

and it is easy to verify that (2.168) yields directly the complex conjugate of this. After quantization, this becomes an equation for the field operator $\psi(\mathbf{x}',t)$, where $\psi^*(\mathbf{x}',t)$ is to be replaced by $\psi^{\dagger *}(\mathbf{x}',t)$, as usual.

Let us also remark that the equation of motion (2.170) can be used directly to derive the n-body Schrödinger equation once more using time-dependent field operators. As a function of time, an arbitrary state vector evolves as follows

$$|\psi(t)\rangle=e^{-i\hat{H}t/\hbar}|\psi(0)\rangle. \tag{2.171}$$

Multiplying this by the basis bra-vectors

$$\frac{1}{\sqrt{n!}}\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \tag{2.172}$$

we obtain the time-dependent Schrödinger wave function

$$\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t). \tag{2.173}$$

Inserting between each pair of $\hat{a}_{\mathbf{x}_\nu}$ operators the trivial unit factors $1=e^{-i\hat{H}t/\hbar}e^{i\hat{H}t/\hbar}$, each of these operators is transformed into the time-dependent field operators $\hat{\psi}(\mathbf{x}_\nu,t)$, and one has

$$\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t)=\frac{1}{\sqrt{n!}}\langle 0|e^{-i\hat{H}t/\hbar}\hat{\psi}(\mathbf{x}_n,t)\cdots\hat{\psi}(\mathbf{x}_1,t)|\psi(0)\rangle \tag{2.174}$$

Using the zero-energy property (2.128) of the vacuum state, this becomes

$$\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t)=\langle\mathbf{x}_1,\ldots,\mathbf{x}_n;t|\psi(0)\rangle. \tag{2.175}$$

The bra states arising from the application of the time-dependent field operators $\hat{\psi}(\mathbf{x}_i,t)$ to the vacuum state on the left,

$$\frac{1}{\sqrt{n!}}\langle 0|\hat{\psi}(\mathbf{x}_n,t)\cdots\hat{\psi}(\mathbf{x}_1,t), \tag{2.176}$$

define a new time-dependent basis

$$\langle\mathbf{x}_1,\ldots,\mathbf{x}_n;t|, \tag{2.177}$$

with the property

$$\langle\mathbf{x}_1,\ldots,\mathbf{x}_n;t|\psi(0)\rangle\equiv\langle\mathbf{x}_1,\ldots,\mathbf{x}_n|\psi(t)\rangle. \tag{2.178}$$

If we apply to the states (2.176) the differential operator (2.170) and use the canonical equal-time commutation rules (2.136), we may derive once more that $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n;t)$ obeys the Schrödinger equation (2.17).

The difference between the earlier form (2.96) and the form (2.175) of defining the wave function is, of course, the second-quantized version of the difference between the Schrödinger and the Heisenberg picture for the ordinary quantum mechanical wave functions. In Eq. (2.96), the states $|\psi(t)\rangle$ are *time-dependent* but the basis ket vectors $\langle\mathbf{x}_1,..,\mathbf{x}_n|$ are not, and with them also the field operators $\hat{\psi}(\mathbf{x},0)=\hat{a}_{\mathbf{x}}$ generating them. In Eq. (2.175), on the contrary, the states $\langle\psi(0)|$ are *time-independent* (and may be called Heisenberg states), but the local basis bra states $\langle\mathbf{x}_1,\ldots,\mathbf{x}_n;t|$ are not, and with them the field operators $\hat{\psi}(\mathbf{x},t)$ generating it. Whatever representation we use, the n-body wave function $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n,t)$ is always in the Schrödinger representation. The change of picture concerns only the operator structure of the many-particle description.

Certainly, there is also the possibility of changing the picture for the $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n,t)$ wave functions but this unitary transformation would take place in another Hilbert space, namely in the space of square integrable functions of n arguments where $\hat{p}$ and $\hat{x}$ are the differential operators $-i\hbar\partial_{\mathbf{x}}$ and $\mathbf{x}$.

When going through the latter alternative proof that (2.175) satisfies the n-body Schrödinger equation we realize that at no place we need the assumption of time-independent potentials. Thus we can conclude that the canonical quantization scheme for the action (2.159) is valid for an arbitrary explicit time dependence of the potentials in $\hat{H}$ [see (2.5)] and is always equivalent to the Schrödinger description for an arbitrary number of particles.

2.9 More General Creation and Annihilation Operators

In many applications it is possible to solve the Schrödinger equation with only the one-body potential $V_1(\mathbf{x};t)$ exactly. Then it is useful to employ, instead of the creation and annihilation operators of particles at a point, another equivalent set of such operators which refers right-away to the corresponding eigenstates. We do this by expanding the field operator into the complete set of solutions of the one-particle Schrödinger equation

$$\hat{\psi}(\mathbf{x},t)=\sum_\alpha \psi_{E_\alpha}(\mathbf{x},t)\hat{a}_\alpha. \tag{2.179}$$

If the one-body potential is time independent and there is no two-body potential, the states have the time dependence

$$\psi_{E_\alpha}(\mathbf{x},t)=\psi_{E_\alpha}(\mathbf{x})\,e^{-iE_\alpha t/\hbar}. \tag{2.180}$$

The expansion (2.179) is inverted to give

$$\hat{a}_\alpha=\int d^3x\,\psi^*_{E_\alpha}(\mathbf{x},t)\hat{\psi}(\mathbf{x},t), \tag{2.181}$$

which we shall write shorter in a scalar-product notation as

$$\hat{a}_\alpha=(\psi_{E_\alpha}(t),\hat{\psi}(t)). \tag{2.182}$$

As opposed to the bra-ket notation to denote basis-independent scalar products, the parentheses indicate more specifically a scalar product between spatial wave functions.

From the commutation rules (2.136) we find that the new operators $\hat{a}_\alpha$, $\hat{a}^\dagger_\alpha$ satisfy the commutation rules

$$\begin{aligned}
[\hat{a}_\alpha,\hat{a}_{\alpha'}] &= [\hat{a}^\dagger_\alpha,\hat{a}^\dagger_{\alpha'}]=0,\\
[\hat{a}_\alpha,\hat{a}^\dagger_{\alpha'}] &= \delta_{\alpha,\alpha'}.
\end{aligned} \tag{2.183}$$

Inserting (2.179) into (2.137) with $V_2=0$, we may use the orthonormality relation among the one-particle states $\psi_{E_\alpha}(\mathbf{x})$ to find the field operator representation for the Hamilton operator

$$\hat{H}=\sum_\alpha E_\alpha\hat{a}^\dagger_\alpha\hat{a}_\alpha. \tag{2.184}$$

The eigenstates of the time-independent Schrödinger equation

$$\hat{H}|\psi(t)\rangle = E|\psi(t)\rangle \tag{2.185}$$

are now

$$|n_1, \dots, n_n\rangle = \frac{1}{\sqrt{n_1! \cdots n_n!}} (\hat{a}^\dagger_{\alpha_1})^{n_1} \cdots (\hat{a}^\dagger_{\alpha_k})^{n_k} |0\rangle, \tag{2.186}$$

where the prefactor ensures the proper normalization. The energy is

$$E = \sum_{i=1}^{k} E_{\alpha_i} n_i. \tag{2.187}$$

Finally, by forming the scalar products

$$\frac{1}{\sqrt{n!}} \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} (\hat{a}^\dagger_{\alpha_1})^{n_1} \cdots (\hat{a}^\dagger_{\alpha_k})^{n_k} |0\rangle \frac{1}{\sqrt{n_1! \cdots n_k!}}, \tag{2.188}$$

we recover precisely the symmetrized wave functions (2.29) with the normalization factors (2.38).

Similar considerations are, of course, possible in the Heisenberg picture of the operators $\hat{a}^\dagger_\alpha$, $\hat{a}_\alpha$ which can be obtained from

$$\hat{a}_\alpha(t) = \int d^3x \psi^*_{E_\alpha}(\mathbf{x}) \hat{\psi}(\mathbf{x}, t). \tag{2.189}$$

In the field operator description of many-body systems, the Schrödinger wave function $\psi(\mathbf{x}, t)$ has become a canonically quantized field object. Oberserve that the field $\psi(\mathbf{x}, t)$ by itself contains all relevant quantum mechanical information of the system via the derivative terms of the action (2.159),

$$\hat{\psi}^\dagger(\mathbf{x}, t) i\hbar\partial_t \hat{\psi}(\mathbf{x}, t) + \frac{\hbar^2}{2M} \hat{\psi}^\dagger(\mathbf{x}, t) \partial^2_{\mathbf{x}} \hat{\psi}(\mathbf{x}, t). \tag{2.190}$$

This fixes the relation between wavelength and momentum and between frequency and energy. The field quantization which introduces the additional processes of particle creation and annihilation is distinguished from this and often referred to as *second quantization.*

It should be kept in mind that for a given n-body system, second quantization is completely equivalent and does not go beyond the usual n-body Schrödinger theory. It merely introduces a technical advantage of collecting the wave equations for any particle number n into a single operator representation. This advantage is, nevertheless, of great use in treating systems with many identical particles. In the limit of large particle densities, it gives rise to approximations which in the Schrödinger formulation would be very difficult to reproduce. In particular, collective excitations of many-particle systems find their easiest explanation in terms of a quantum field formulation.

The full power of quantum fields, however, will unfold itself when trying to explain the physics of relativistic particles, where the number of particles is no longer conserved. Since the second-quantized Hilbert space contains any number of particles, the second-quantized formulation allows naturally for the description of the emission and absorption of fundamental particles, processes which the Schrödinger equation is unable to deal with.

2.10 Quantum Field Formulation of Many-Fermion Schrödinger Equations

The question arises whether an equally simple formalism can be found which automatically leads to the correct antisymmetric many-particle states

$$|\mathbf{x}_1,\ldots,\mathbf{x}_n\rangle^A = \frac{1}{\sqrt{n!}}\sum_P \epsilon_P |\mathbf{x}_{p(1)}\rangle \otimes \ldots \otimes |\mathbf{x}_{p(n)}\rangle. \tag{2.191}$$

This is indeed possible. Let us remember that the symmetry of the wave functions was a consequence of the commutativity of the operators $\hat{\psi}(\mathbf{x},t)$ for different position values $\mathbf{x}$ Obviously, we can achieve an antisymmetry in the coordinates by forming product states

$$|\mathbf{x}_1,\ldots,\mathbf{x}_n\rangle^A = \frac{1}{\sqrt{n!}}\hat{a}^\dagger_{\mathbf{x}_1}\cdots\hat{a}^\dagger_{\mathbf{x}_n}|0\rangle \tag{2.192}$$

and requiring anticommutativity of the particle creation and annihilation operators:

$$\{\hat{a}^\dagger_{\mathbf{x}},\hat{a}^\dagger_{\mathbf{x}'}\} = 0, \qquad \{\hat{a}_{\mathbf{x}},\hat{a}_{\mathbf{x}'}\} = 0. \tag{2.193}$$

The curly bracket denotes the anticommutator defined in Eq. (2.108). To define a closed algebra, we require in addition as an analog of the third commutation rule (2.72) for bosons the anticommutation rule

$$\{\hat{a}_{\mathbf{x}},\hat{a}^\dagger_{\mathbf{x}'}\} = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{2.194}$$

As in the bosonic case we introduce a vacuum state $|0\rangle$ which is normalized as in (2.84) and contains no particle [cf. (2.83)]:

$$\hat{a}_{\mathbf{x}}|0\rangle = 0\ ,\ \ \langle 0|\hat{a}^\dagger_{\mathbf{x}} = 0. \tag{2.195}$$

The anticommutation rules (2.193) have the consequence that each point can at most be occuoied by a single particle. Indeed, applying the creation operator twice to the vacuum state yields zero:

$$\hat{a}^\dagger_{\mathbf{x}}\hat{a}^\dagger_{\mathbf{x}}|0\rangle = \{\hat{a}^\dagger_{\mathbf{x}},\hat{a}^\dagger_{\mathbf{x}}\}|0\rangle - \hat{a}^\dagger_{\mathbf{x}}\hat{a}^\dagger_{\mathbf{x}}|0\rangle = 0. \tag{2.196}$$

This gurantees the validity of the *Pauli exclusion priceiple*.

The properties (2.193), (2.194), and (2.195) are sufficient to derive the many-body Schrödinger equations with two-body interactions for an arbitrary number of fermionic particles. It is easy to verify that the second-quantized Hamiltonian has the same form as in Eq. (2.127). The proof proceeds along the same line as in the symmetric case, Eqs. (2.91)–(2.127). A crucial tool is the operator chain rules (2.109) derived for anticommutators. The minus sign by which anticommutators differ from commutators cancels out in all relevant equations.

As for bosons we define a time-dependent quantum field for fermions in the Heisenberg picture as

$$\begin{aligned}\hat{\psi}(\mathbf{x},t) &= e^{i\hat{H}t/\hbar}\hat{\psi}(\mathbf{x},0)e^{-i\hat{H}t/\hbar}\\ &= e^{i\hat{H}t/\hbar}\hat{a}_{\mathbf{x}}e^{-i\hat{H}t/\hbar},\end{aligned} \tag{2.197}$$

and find equal-time anticommutation rules of the same type as the commutation relations (2.136):

$$\begin{aligned}\{\hat{\psi}(\mathbf{x},t),\hat{\psi}(\mathbf{x}',t)\} &= 0,\\ \{\hat{\psi}^\dagger(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\} &= 0,\\ \{\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\} &= \delta^{(3)}(\mathbf{x}-\mathbf{x}').\end{aligned} \tag{2.198}$$

The Hamiltonian has again the form Eq. (2.137).

There is only one place where the fermionic case is not completely analogous to the bosonic one: The second-quantized formulation cannot be derived from a standard canonical formalism of an infinite number of generalized coordinates. The standard formalism of quantum mechanics applies only to true physical canonical coordinates $p(t)$ and $q(t)$, and these can never account for anticommuting properties of field variables.[3] Thus an identification analogous to (2.142),

$$\hat{p}_{\mathbf{x}}(t) \equiv \hat{\psi}_I(\mathbf{x},t), \qquad \hat{q}_{\mathbf{x}}(t) \equiv \hat{\psi}_R(\mathbf{x},t), \tag{2.199}$$

is at first impossible.

The canonical formalism may nevertheless be generalized appropriately. We may start out with exactly the same classical Lagrangian as in the boson case, Eq. (2.160), but treat the fields formally as anticommuting objects, i.e.,

$$\psi(\mathbf{x},t)\psi(\mathbf{x}',t') = -\psi(\mathbf{x}',t')\psi(\mathbf{x},t). \tag{2.200}$$

In mathematics, such objects are called *Grassmann variables*. Using these, we define again classical canonical momenta

$$p_{\mathbf{x}}(t) \equiv \frac{\delta L}{\delta\psi(\mathbf{x},t)} = -i\hbar\psi^\dagger(\mathbf{x},t) \equiv \pi(\mathbf{x},t). \tag{2.201}$$

Together with the field variable $q_{\mathbf{x}}(t) = \psi^\dagger(\mathbf{x},t)$, this is postulated to satisfy the canonical anticommutation rule

$$\{p_{\mathbf{x}}(t), q_{\mathbf{x}'}(t)\} = -i\hbar\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{2.202}$$

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[3] For a detailed discussion of classical machanics with supersymmetric Lagrange coordinates see A. Kapka, *Supersymmetrie*, Teubner, 1997

2.11 Free Nonrelativistic Particles and Fields

An important way to approach interacting theories will be based on perturbative methods. Usually, these begin with the free theory and prescribe how to calculate successive corrections due to the interaction energies. A detailed discussion of how and when this works will be given later. It seems intuitively obvious, however, that at least for weak interactions, the free theory may be a good starting point for an approximation scheme. It is therefore worthwhile to study a few properties of the free theory in detail.

The free-field action is, according to Eqs. (2.159) and (2.137) for $V_1(\mathbf{x}) = 0$ and $V_2(\mathbf{x}-\mathbf{x}') = 0$:

$$\mathcal{A} = \int dt d^3x\, \psi^*(\mathbf{x},t) \left[i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2 \right] \psi(\mathbf{x},t). \tag{2.203}$$

The quantum field $\hat{\psi}(\mathbf{x},t)$ satisfies the field operator equation

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 \right) \hat{\psi}(\mathbf{x},t) = 0, \tag{2.204}$$

with the conjugate field satisfying

$$\hat{\psi}^\dagger(x,t) \left(-i\hbar \overleftarrow{\partial}_t + \frac{\hbar^2}{2M} \overleftarrow{\partial}_{\mathbf{x}}^2 \right) = 0. \tag{2.205}$$

The equal-time commutation rules for bosons and fermions are

$$\begin{aligned} [\hat{\psi}(\mathbf{x},t), \hat{\psi}(\mathbf{x}',t)]_\mp &= 0, \\ [\hat{\psi}^\dagger(\mathbf{x},t), \hat{\psi}^\dagger(\mathbf{x}',t)]_\mp &= 0, \\ [\hat{\psi}(\mathbf{x},t), \hat{\psi}^\dagger(\mathbf{x}',t)]_\mp &= \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \end{aligned} \tag{2.206}$$

where we have denoted commutator and anticommutator collectively by $[\dots, \dots]_\mp$, respectively.

In a finite volume V, the solutions of the free one-particle Schrödinger equation are given by the time-dependent version of the plane wave functions (1.111) [compare (2.180)]:

$$\psi_{\mathbf{p}^{\mathbf{m}}}(\mathbf{x},t) = \frac{1}{\sqrt{V}} \exp\left\{ \frac{i}{\hbar} \left(\mathbf{p}^{\mathbf{m}}\mathbf{x} - \frac{\mathbf{p}^{\mathbf{m}2}}{2M}t \right) \right\}. \tag{2.207}$$

These are orthonormal in the sense

$$\int d^3x\, \psi^*_{\mathbf{p}^{\mathbf{m}}}(\mathbf{x},t)\psi_{\mathbf{p}^{\mathbf{m}'}}(\mathbf{x},t) \;=\; \delta_{\mathbf{p}^{\mathbf{m}},\mathbf{p}^{\mathbf{m}'}}, \tag{2.208}$$

and complete, as expressed by

$$\sum_{\mathbf{p}^{\mathbf{m}}} \psi_{\mathbf{p}^{\mathbf{m}}}(\mathbf{x},t)\psi^*_{\mathbf{p}^{\mathbf{m}}}(\mathbf{x}',t) = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{2.209}$$

valid inside the finite volume V. As in Eq. (2.179) we now expand the field operator in terms of these solution as

$$\hat{\psi}(\mathbf{x},t) = \sum_{\mathbf{p}^{\mathbf{m}}} \psi_{\mathbf{p}^{\mathbf{m}}}(\mathbf{x},t)\hat{a}_{\mathbf{p}^{\mathbf{m}}}. \tag{2.210}$$

This expansion is inverted with the help of the scalar product (2.182) as

$$\hat{a}_{\mathbf{p}^{\mathbf{m}}} = (\psi_{\mathbf{p}^{\mathbf{m}}}(t), \hat{\psi}(t)) = \int d^3x\, \psi^*_{\mathbf{p}^{\mathbf{m}}}(\mathbf{x},t)\hat{\psi}(\mathbf{x},t). \tag{2.211}$$

In the sequel we shall usually omit the superscript of the momenta $\mathbf{p}^{\mathbf{m}}$ if their discrete nature is evident from the context. The operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}^\dagger_{\mathbf{p}}$, obey the canonical commutation rules corresponding to Eq. (2.183):

$$\begin{aligned}
[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}]_\mp &= 0, \\
[\hat{a}^\dagger_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}'}]_\mp &= 0, \\
[\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}'}]_\mp &= (2\pi\hbar)^3\, \delta^{(3)}(\mathbf{p}-\mathbf{p}') \equiv \delta^{(3)}(\mathbf{p}-\mathbf{p}'),
\end{aligned} \tag{2.212}$$

where we have used the modified δ-functions introduced in Eq. (1.122).

In an infinite volume, we use the time-dependent version of the continous wave functions (1.120)

$$\psi_{\mathbf{p}}(\mathbf{x},t) = \exp\left\{\frac{i}{\hbar}\left(\mathbf{p}\mathbf{x} - \frac{\mathbf{p}^2}{2M}t\right)\right\}, \tag{2.213}$$

which are orthonormal in the sense

$$\begin{aligned}
\int d^3x\, \psi^*_{\mathbf{p}}(\mathbf{x},t)\psi_{\mathbf{p}'}(\mathbf{x},t) &= (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{p}') \\
&\equiv \delta^{(3)}(\mathbf{p}-\mathbf{p}'),
\end{aligned} \tag{2.214}$$

and complete, as expressed by

$$\int \frac{d^3p}{(2\pi\hbar)^3}\, \psi_{\mathbf{p}}(\mathbf{x},t)\psi^*_{\mathbf{p}}(\mathbf{x}',t) \equiv \int d^3p\, \psi_{\mathbf{p}}(\mathbf{x},t)\psi^*_{\mathbf{p}}(\mathbf{x}',t) = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{2.215}$$

In terms of these continuum wave functions, we expand the field operator as

$$\hat{\psi}(\mathbf{x},t) = \int d^3p\, \psi_{\mathbf{p}}(\mathbf{x},t)\hat{a}(\mathbf{p}), \tag{2.216}$$

and have the inverse

$$\hat{a}(\mathbf{p}) = (\psi_{\mathbf{p}}(t), \hat{\psi}(t)) = \int d^3x\, \psi^*_{\mathbf{p}}(\mathbf{x},t)\hat{\psi}(\mathbf{x},t). \tag{2.217}$$

The discrete-momentum operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}^\dagger_{\mathbf{p}}$ and the continuous ones $\hat{a}(\mathbf{p})$ and $\hat{a}^\dagger(\mathbf{p})$ are related by [recall Eq. (1.116)]

$$\hat{a}(\mathbf{p}) = \sqrt{V}\hat{a}_{\mathbf{p}}, \qquad \hat{a}^\dagger(\mathbf{p}) = \sqrt{V}\hat{a}^\dagger_{\mathbf{p}}. \tag{2.218}$$

For the continuous-momentum operators $\hat{a}(\mathbf{p})$ and $\hat{a}(\mathbf{p})^\dagger$, the canonical commutation rules Eq. (2.183) take the form

$$\begin{aligned}
[\hat{a}(\mathbf{p}),\hat{a}(\mathbf{p}')]_\mp &= 0,\\
[\hat{a}^\dagger(\mathbf{p}),\hat{a}^\dagger(\mathbf{p}')]_\mp &= 0,\\
[\hat{a}(\mathbf{p}),\hat{a}^\dagger(\mathbf{p}')]_\mp &= \delta^{(3)}(\mathbf{p}-\mathbf{p}'). \qquad (2.219)
\end{aligned}$$

The time-independent many-particle states are obtained by repeatedly applying as in (2.186) any number of creation operators $\hat{a}^\dagger_{\mathbf{p}}$ [or $\hat{a}^\dagger(\mathbf{p})$] to the vacuum state $|0\rangle$, thus creating states

$$|n_1,n_2,\dots,n_k\rangle = \mathcal{N}^{S,A}(\hat{a}^\dagger_{\mathbf{p}_1})^{n_1}\cdots(\hat{a}^\dagger_{\mathbf{p}_k})^{n_k}|0\rangle, \qquad (2.220)$$

where the normalization factor is determined as in Eq. (2.186). For bosons with n_1 identical states of momentum p_1, with n_2 identical states of momentum p_2, etc., the normalization factor is

$$\mathcal{N}^S = \frac{1}{\sqrt{n_1!\cdots n_k!}}. \qquad (2.221)$$

The same formula can be used for fermions only that then n_i can only take the values 0 or 1, so that $\mathcal{N}^A \equiv 1$. The time-independent wave functions are obtained as

$$\psi_E^{S,A}(\mathbf{x}_1,\dots,\mathbf{x}_n) = \frac{\mathcal{N}^{S,A}}{\sqrt{n!}}\langle 0|\hat{\psi}(\mathbf{x}_n,0)\cdots\hat{\psi}(\mathbf{x}_1,0)(\hat{a}^\dagger_{\mathbf{p}_1})^{n_1}\cdots(\hat{a}^\dagger_{\mathbf{p}_k})^{n_k}|0\rangle, \qquad (2.222)$$

and the time-dependent ones as

$$\begin{aligned}
\psi^{S,A}(\mathbf{x}_1,\dots,\mathbf{x}_n;t) &= \psi_E^{S,A}(\mathbf{x}_1,\dots,\mathbf{x}_n)e^{-iEt/\hbar} \qquad (2.223)\\
&= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}}\langle 0|\hat{\psi}(\mathbf{x}_n,0)\cdots\hat{\psi}(\mathbf{x}_1,0)e^{-i\hat{H}t/\hbar}(\hat{a}^\dagger_{\mathbf{p}_1})^{n_1}\dots(\hat{a}^\dagger_{\mathbf{p}_k})^{n_k}|0\rangle\\
&= \frac{\mathcal{N}^{S,A}}{\sqrt{n!}}\langle 0|\hat{\psi}(\mathbf{x}_n,0)\cdots\hat{\psi}(\mathbf{x}_1,0)[\hat{a}^\dagger_{\mathbf{p}_1}(t)]^{n_1}\cdots[\hat{a}^\dagger_{\mathbf{p}_k}(t)]^{n_k}|0\rangle,
\end{aligned}$$

with the time-dependent creation operators being defined by

$$\hat{a}^\dagger_{\mathbf{p}}(t) \equiv e^{i\hat{H}t/\hbar}\hat{a}^\dagger_{\mathbf{p}}e^{-i\hat{H}t/\hbar}. \qquad (2.224)$$

The energy of the states (2.220) is

$$E = \sum_{i=1}^{k} n_i E_{\mathbf{p}_i}. \qquad (2.225)$$

The states (2.220) form the so-called *occupation number basis* of the Hilbert space. For fermions, n_i can only be 0 or 1, due to the anticommutativity of the operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}^\dagger_{\mathbf{p}}$ among themselves. The basis states are properly normalized

$$\langle n_1n_2n_3\dots n_k|n'_1n'_2n'_3\dots n'_k\rangle = \delta_{n_1n'_1}\delta_{n_2n'_2}\delta_{n_3n'_3}\cdots\delta_{n_kn'_k}, \qquad (2.226)$$

and satisfy the completeness relation

$$\sum_{n_1 n_2 n_3 \dots n_k} |n_1 n_2 n_3 \dots n_k\rangle\langle n_1 n_2 n_3 \dots n_k| = 1^{S,A}, \tag{2.227}$$

where the unit operator on the right-hand side covers only the physical Hilbert space of symmetric or antisymmetric n-body wave functions.

2.12 Second-Quantized Current Conservation Law

In Section 1.1 we have observed as an essential property for the probability interpretation of the Schrödinger wave functions that the probability density (1.3) and the probability current density (1.29) were related by the local conservation law Eq. (1.30):

$$\partial_t \rho(\mathbf{x}, t) = -\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{x}, t). \tag{2.228}$$

This followed directly from the Schrödinger equation (2.170). Since the same equation holds for the field operators, i.e., with $\psi^*(\mathbf{x}', t)$ replaced by $\hat{\psi}^\dagger(\mathbf{x}', t)$, the field operators of charge and current density

$$\begin{aligned} \hat{\rho}(\mathbf{x}, t) &= \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t), \\ \hat{\mathbf{j}}(\mathbf{x}, t) &= -i\frac{\hbar}{2M}\hat{\psi}^\dagger(\mathbf{x}, t) \overset{\leftrightarrow}{\boldsymbol{\nabla}} \hat{\psi}(\mathbf{x}, t) \end{aligned} \tag{2.229}$$

satisfy the same relation. When integrating (2.228) over all space as in Eq. (1.32), the resulting global conservation law ensures the time independence of the operator

$$\hat{N} = \int d^3x \, \hat{\rho}(\mathbf{x}, t) = \int d^3x \, \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t). \tag{2.230}$$

Being time-independent we can use (2.132) to rewrite

$$\hat{N} = \int d^3x \, \hat{\rho}(\mathbf{x}, 0) = \int d^3x \, \hat{\psi}^\dagger(\mathbf{x}, 0)\hat{\psi}(\mathbf{x}, 0) = \int d^3x \, \hat{a}^\dagger_{\mathbf{x}}\hat{a}_{\mathbf{x}}, \tag{2.231}$$

so that $\hat{N}$ coincides with the particle number operator (2.75). The original form (2.230) is the Heisenberg picture of the particle number operator, which coincides because of (2.231) with the Schrödinger picture since the particle number is conserved.

2.13 Free-Particle Propagator

The perturbation theory of interacting fields to be developed later in Chapter 8) requires knowledge of an important free-field quantity called the *free-particle propagator*. It is the vacuum expectation of the time-ordered product of two free field operators. As we shall see, the calculation of any observable quantities can be reduced to the calculation of some linear combination of products of free propagators [see Section 5.12.1]. Let us first extend the definition (1.145) of the time-ordered product of n time-dependent operators to allow for fermion field operators. Suppose that the times in an operator product $\hat{A}_n(t_n)\cdots\hat{A}_1(t_1)$ have an order

$$t_{i_n} > t_{i_{n-1}} > \ldots > t_{i_1}. \tag{2.232}$$

Then the time-ordered product of the operators is defined by

$$\hat{T}\hat{A}_n(t_n)\cdots\hat{A}_1(t_1) \equiv \epsilon_P \hat{A}_{i_n}(t_{i_n})\cdots\hat{A}_{i_1}(t_{i_1}). \tag{2.233}$$

With respect to the definition (1.146), the right hand side carries a sign factor $\epsilon_P = \pm 1$ depending on whether an even or an odd permutation P of the fermion field operators is necessary to reach the time-ordered form. For bosons, $\varepsilon_P \equiv 1$.

The definition of the time-ordered products can be given more concisely using the Heaviside $\Theta(t)$ function (1.215). For two operators, we have

$$\hat{T}\hat{A}(t_1)\hat{B}(t_2) = \Theta(t_1-t_2)\hat{A}(t_1)\hat{B}(t_2) \pm \Theta(t_2-t_1)\hat{B}(t_2)\hat{A}(t_1), \tag{2.234}$$

with the upper and lower sign applying to bosons and fermions, respectively. The free-particle propagator can now be constructed from the field operators as the vacuum expectation value

$$G(\mathbf{x},t;\mathbf{x}',t') = \langle 0|\hat{T}\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')|0\rangle. \tag{2.235}$$

Applying the free-field operator equations (2.204), (2.205) we derive a remarkable property: The free-particle propagator $G(\mathbf{x},t;\mathbf{x}',t')$ coincides with the *Green function* of the Schrödinger differential operator. Recall that a Green function of a homogeneous differential equation is defined by being the solution of the inhomogeneous equation with a δ-function source (see Section 1.5). This property may easily be verified for the free-particle propagator, which satisfies the differential equation

$$\begin{aligned}
\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)G(\mathbf{x},t;\mathbf{x}',t') &= i\hbar\delta(t-t')\delta^{(3)}(\mathbf{x}-\mathbf{x}'), &(2.236)\\
G(\mathbf{x},t;\mathbf{x}',t')\left(-i\hbar\overleftarrow{\partial}_{t'} + \frac{\hbar^2}{2M}\overleftarrow{\partial}_{\mathbf{x}}^2\right) &= i\hbar\delta(t-t')\delta^{(3)}(\mathbf{x}-\mathbf{x}'), &(2.237)
\end{aligned}$$

thus being a Green function of the free-particle Schrödinger equation: The right-hand side follows directly from the fact that the field $\hat{\psi}(\mathbf{x},t)$ satisfies the Schrödinger equation and the obvious formula

$$\partial_t\Theta(t-t') = \delta(t-t'). \tag{2.238}$$

With the help of the chain rule of differentiation and Eq. (2.234), we see that

$$\begin{aligned}
&\left(i\hbar\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2\right)\langle 0|\hat{T}\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')|0\rangle\\
&\quad= i\hbar\left[\partial_t\Theta(t-t')\langle 0|\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')|0\rangle \pm \partial_t\Theta(t'-t)\langle 0|\hat{\psi}^\dagger(\mathbf{x}',t')\hat{\psi}(\mathbf{x},t)|0\rangle\right]\\
&\quad= i\hbar\delta(t-t')\langle 0|[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)]_\mp|0\rangle = i\hbar\delta(t-t')\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \qquad (2.239)
\end{aligned}$$

where the commuation and anticommutation rules (2.136) and (2.198) have been used, and the unit notmalization (2.84) of the vacuum state.

In the theory of differential equations, Green functions are introduced to find solutions for arbitrary inhomogeneous terms, since such a term can be viewed as a superposition of δ-function sources. In quantum field theory, the same Green functions serve as propagators in solving inhomogeneous differential equations involving *field operators.*

Explicitly, the free field propagator is calculated as follows: Since $\hat{\psi}(\mathbf{x},t)$ annihilates the vacuum, only the first term in the definition Eq. (2.234) contributes so that we can write

$$G(\mathbf{x},t;\mathbf{x}',t') = \Theta(t-t')\langle 0|\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')|0\rangle. \tag{2.240}$$

Inserting the expansion Eq. (2.216) with the wave functions (2.213) and using (2.219), the right-hand side becomes

$$\begin{aligned}&\Theta(t-t')\int \bar{d}^3p\, \bar{d}^3p'\, e^{i[(\mathbf{p}\mathbf{x}-\mathbf{p}'\mathbf{x}')-(\mathbf{p}^2t/2M-\mathbf{p}'^2t'/2M)]/\hbar}\langle 0|\hat{a}(\mathbf{p})\hat{a}^\dagger(\mathbf{p}')|0\rangle\\ &\quad= \Theta(t-t')\int \bar{d}^3p\, e^{i[\mathbf{p}(\mathbf{x}-\mathbf{x}')-\mathbf{p}^2(t-t')/2M]/\hbar}.\end{aligned} \tag{2.241}$$

By completing the square and using the Gaussian integral

$$\int \bar{d}^3p\, e^{-ap^2/2\hbar} = \frac{1}{\sqrt{2\pi\hbar a}^{3}}, \tag{2.242}$$

we find

$$\begin{aligned}G(\mathbf{x},t;\mathbf{x}',t') &= \Theta(t-t')\frac{1}{\sqrt{2\pi i\hbar(t-t')/M}^{3}}e^{iM(\mathbf{x}-\mathbf{x}')^2/2\hbar(t-t')}\\ &= G(\mathbf{x}-\mathbf{x}',t-t').\end{aligned} \tag{2.243}$$

The right-hand side is recognized as the usual quantum-mechanical Green function of the free-particle Schrödinger equation of Eq. (1.235). Indeed, the factor after $\Theta(t-t')$ is simply the one-particle matrix element of the time evolution operator

$$\begin{aligned}\langle 0|\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')|0\rangle &= \langle 0|\hat{\psi}(\mathbf{x})e^{-i\hat{H}(t-t')/\hbar}\hat{\psi}^\dagger(\mathbf{x}')|0\rangle\\ &= \langle \mathbf{x}|\hat{U}(t,t')|\mathbf{x}'\rangle.\end{aligned} \tag{2.244}$$

This is precisely the expression discussed in Eqs. (1.214)–(1.216). It describes the probability amplitude that a single free particle has propagated from $\mathbf{x}$ to $\mathbf{x}'$ in the time $t-t'>0$. For $t-t'<0$, G vanishes.

There exists a more useful way of writing the Fourier representation of the propagator than that in Eq. (2.241). It is based on the integral representation (1.222) of the Heaviside function:

$$\Theta(t-t') = \int_{-\infty}^{\infty} \bar{d}E\, e^{-iE(t-t')/\hbar}\frac{i\hbar}{E+i\eta}. \tag{2.245}$$

As discussed in general in Eqs. (1.220)–(1.221), the $i\eta$ in the denominator ensures the causality. For $t > t'$, the contour of integration can be closed by an infinite semicircle below picking up the pole at $E = -i\eta$, so that we obtain by the residue theorem

$$\Theta(t-t') = 1, \qquad t > t'. \tag{2.246}$$

For $t < t'$, on the other hand, the contour may be closed above and since there is no pole in the upper half-plane:

$$\Theta(t-t') = 0, \qquad t < t'. \tag{2.247}$$

Relation (2.245) can be generalized to

$$\Theta(t-t')e^{-iE_0(t-t')/\hbar} = \int_{-\infty}^{\infty} dE\, e^{-iE(t-t')/\hbar} \frac{i\hbar}{E - E_0 + i\eta}. \tag{2.248}$$

Using this with $E_0 = \mathbf{p}^2/2M$ we find from (2.241) the integral representation

$$G(\mathbf{x}-\mathbf{x}', t-t') = \int d^3p \int_{-\infty}^{\infty} dE\, e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')/\hbar - iE(t-t')/\hbar} \frac{i\hbar}{E - \mathbf{p}^2/2M + i\eta}. \tag{2.249}$$

In this form we can trivially verify the equations of motion (2.236) and (2.237). This expression agrees, of course, with the quantum mechanical time evolution amplitude (1.228).

The Fourier-transformed propagator

$$\begin{aligned} G(\mathbf{p}, E) &= \int d^3x \int_{-\infty}^{\infty} dt\, e^{-i(\mathbf{p}\mathbf{x}-Et)/\hbar} G(\mathbf{x}, t) \\ &= \frac{i\hbar}{E - \mathbf{p}^2/2M + i\eta} \end{aligned} \tag{2.250}$$

has the property of being singular when the variable E is equal to a physical particle energy $E = \mathbf{p}^2/2M$. This condition is often called the *energy shell* condition. It is a general property of Green functions that their singularities in the energy momentum variables display the spectra of the particles of the system.

2.14 Quantum Statistic of Free Particles

2.14.1 Thermodynamic Quantities

Consider the grand-canonical partition function introduced in Eq. (1.120):

$$Z_G(T, \mu) = \mathrm{Tr}\,(e^{-(\hat{H}-\mu\hat{N})/k_BT}). \tag{2.251}$$

The trace has to be taken over the complete set of basis states (2.220):

$$\sum_{n_1 n_2 n_3} \langle n_1 n_2 n_3 \ldots | e^{-(E_{n_1 n_2 \ldots} - \mu \sum_i n_i)/k_BT} | n_1 n_2 n_3 \ldots \rangle. \tag{2.252}$$

Using the additivity of the energies of all single-particle states found in Eq. (2.225), this can be written as an infinite product

$$Z_G(T,\mu)=\sum_{n_1}e^{-(\frac{\mathbf{p}_1^2}{2M}-\mu)n_1/k_BT}\sum_{n_2}e^{-(\frac{\mathbf{p}_2^2}{2M}-\mu)n_2/k_BT}\sum_{n_3}e^{-(\frac{\mathbf{p}_3^2}{2M}-\mu)n_3/k_BT}\times\dots\,. \tag{2.253}$$

Each factor represents the partition function associated with available single-particle momentum $\mathbf{p}_1,\mathbf{p}_2,\dots$, enumerated by $1,2,3,\dots$. The product is turned into a sum by considering the grand-canonical free energy

$$\begin{aligned} F_G(T,\mu) &\equiv -k_BT\log Z_G(T,\mu) &(2.254)\\ &= -k_BT\sum_{\mathbf{p}}\log\sum_n e^{-(\frac{\mathbf{p}^2}{2M}-\mu)n/k_BT}. &(2.255)\end{aligned}$$

We now distinguish between Bose and Fermi particles. In the first case, the occupation numbers n_i run over all integers $0,1,2,\dots$ up to infinity:

$$\sum_{n=0}^{\infty}e^{-(\frac{\mathbf{p}^2}{2M}-\mu)n/k_BT}=\frac{1}{1-e^{-(\frac{\mathbf{p}^2}{2M}-\mu)/k_BT}}. \tag{2.256}$$

In the second case, n_i can be only zero or one, so that

$$\sum_{n=0}^{1}e^{-(\frac{\mathbf{p}^2}{2M}-\mu)n/k_BT}=1+e^{-(\frac{\mathbf{p}^2}{2M}-\mu)/k_BT}. \tag{2.257}$$

Combining both results we arrive at

$$F_G(T,\mu)=\pm k_BT\sum_{\mathbf{p}}\log[1\mp e^{-(\frac{\mathbf{p}^2}{2M}-\mu)/k_BT}]. \tag{2.258}$$

In a large volume, the sum over momentum states may be turned into an integral with the help of the standard formula

$$\sum_{\mathbf{p}}\longrightarrow gV\int\frac{d^3p}{(2\pi\hbar)^3}=gV\int \bar{d}^3p. \tag{2.259}$$

In writing this we have allowed for a degeneracy number g for each momentum state $\mathbf{p}$ accounting for a possible number of internal degrees of freedom of each state. In the absence of internal quantum numbers the different spin polarization states have to be counted properly, i.e.

$$g=2s+1 \tag{2.260}$$

where s is the spin of the particles.

As an alternative to the momentum integral (2.259), we may integrate over the single-particle energies. With the energy $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2M$, the relation between the integration measures is

$$\begin{aligned}\int d^3p &= \frac{4\pi}{(2\pi)^3\hbar^3}\int_0^\infty dp\,p^2 \\ &= \frac{1}{\sqrt{2\pi\hbar^2/M}^3}\frac{2}{\sqrt{\pi}}\int_0^\infty d\varepsilon\sqrt{\varepsilon} \equiv \int N_\varepsilon d\varepsilon,.\end{aligned} \tag{2.261}$$

In the last expression we have introduced the quantity

$$N_\varepsilon \equiv \frac{1}{\sqrt{2\pi\hbar^2/M}^3}\frac{2}{\sqrt{\pi}}\sqrt{\varepsilon}, \tag{2.262}$$

which is the *density of states* per unit energy interval and volume. With the help of this quantity, we may write

$$F_G(T,\mu,V) = gV\int_0^\infty d\varepsilon N_\varepsilon F_\varepsilon(T,\mu) \tag{2.263}$$

where

$$F_\varepsilon(T,\mu) = \pm k_BT\log[1 \mp e^{-(\varepsilon-\mu)/k_BT}] \tag{2.264}$$

are the grand-canonical free energies of the individual single-particle energy shells.

According to the thermodynamic rule (1.272), the average particle number is found from the derivative of $F_G(T,\mu,V)$ with respect to the chemical potential. Using the integral representation (2.263), we find

$$\begin{aligned}N &= -gV\int_0^\infty d\varepsilon N_\varepsilon \frac{\partial}{\partial\mu}F_\varepsilon(T,\mu) \\ &\equiv gV\int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon,\end{aligned} \tag{2.265}$$

where

$$n_\varepsilon \equiv -\frac{\partial}{\partial\mu}F_\varepsilon(T,\mu) = \frac{1}{e^{(\varepsilon-\mu)/k_BT} \mp 1} \tag{2.266}$$

are the average Bose and Fermi occupation numbers of a level of energy ε, respectively. They are plotted in Figs. 2.1 and 2.2.

The internal energy of the system can be calculated as follows

$$\begin{aligned}E &= \int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon \varepsilon \\ &= g\frac{V}{\sqrt{2\pi\hbar^2/M}^3}\frac{2}{\sqrt{\pi}}\int_0^\infty \frac{d\varepsilon\varepsilon^{3/2}}{e^{(\varepsilon-\mu)/k_BT} \mp 1}.\end{aligned} \tag{2.267}$$

On the other hand, we find by a partial integration of (2.267) with respect to the energy that the grand-canonical partition function can be rewritten as

$$F_G(T,\mu,V) = \int_0^\infty d\varepsilon N_\varepsilon F_\varepsilon = -\frac{2}{3}\int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon \varepsilon. \tag{2.268}$$

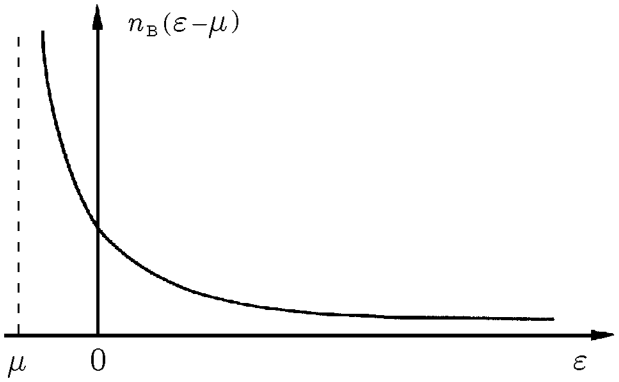

FIGURE 2.1 Average Bose occupation number $n_B(\varepsilon - \mu)$. Note that free bosons have a negative chemical potential μ.

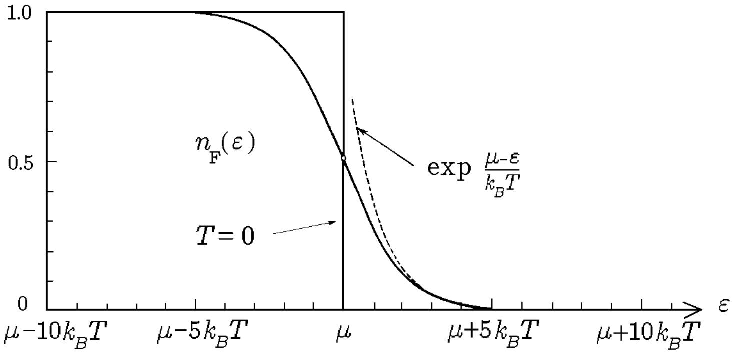

FIGURE 2.2 Average Fermi occupation number $n_F(\varepsilon)$. Fermions have a positive chemical potential μ.

This implies the general thermodynamic relation for a free Bose or Fermi gas:

$$F_G = -\frac{2}{3}E. \tag{2.269}$$

Recalling the definition of the pressure (1.299), we have thus found the *equation of state* for a free Bose or Fermi gas:

$$pV = \frac{2}{3}E. \tag{2.270}$$

Using in (2.267) the variable $z \equiv \varepsilon/k_BT$ we can write (2.265) as

$$N = N(T, \mu) \equiv g\frac{V}{\lambda^3(T)}\frac{2}{\sqrt{\pi}}I^{\mp}_{3/2}\left(\frac{\mu}{k_BT}\right), \tag{2.271}$$

where

$$\lambda(T) \equiv \frac{1}{\sqrt{2\pi\hbar^2/Mk_BT}} \tag{2.272}$$

is the *thermal lenght scale* associated with the mass M and the temperature T, and we have introduced the functions

$$I_n^{\mp}(\alpha) \equiv \int_0^\infty dz \frac{z^{n-1}}{e^{z-\alpha} \mp 1}. \tag{2.273}$$

After expanding the denominator in a power series, we can perform the integrals and find for bosons an infinite sum

$$I_n^-(\alpha) = \Gamma(n) \sum_{k=1}^{\infty} \frac{e^{k\alpha}}{k^n}. \tag{2.274}$$

The sum converges only for $\alpha < 0$. In the limit $\alpha \to -0$, it has the limit

$$I_n^-(0) = \Gamma(n)\zeta(n), \qquad n > 1. \tag{2.275}$$

where $\zeta(n)$ is Riemann's zeta function

$$\zeta(\nu) \equiv \sum_{k=1}^{\infty} \frac{1}{k^\nu}. \tag{2.276}$$

For $n \leq 1$, $I_n^-(\alpha)$ diverges like $(-\alpha)^{n-1}$ for $\alpha \to -0$. In the opposite limit $\alpha \to -\infty$, it goes to a constant

$$I_n^-(\alpha) \to e^\alpha \Gamma(n). \tag{2.277}$$

This limit is needed to find the high-temperature behavior of the bosons at a fixed average particle number N, as we see from Eq. (2.271). For large T, μ/k_BT diverhes to $-\infty$.

For fermions, the expansion (2.274) reads

$$I_n^+(\alpha) = \Gamma(n) \sum_{k=1}^{\infty} (-1)^{n-1} \frac{e^{k\alpha}}{k^n}, \tag{2.278}$$

the only difference being the alternating signs. For $\alpha = 0$, this becomes

$$I_n^+(0) = \frac{1}{1} - \frac{1}{2^n} + \frac{1}{3^n} - \frac{1}{4^n} + \ldots = \sum_{k=0}^{\infty} \frac{1}{k^n} - 2^{1-n} \sum_{k=0}^{\infty} \frac{1}{k^n} = \left(1 - 2^{1-n}\right)\zeta(n). \tag{2.279}$$

For constant N, the chemical potential changes with the temperature in a way determined by the vanishing of the derivative of (2.271), which yields the equation

$$T\partial_T \frac{\mu}{k_BT} = -3 \frac{I_{3/2}(\frac{\mu}{k_BT})}{I_{1/2}(\frac{\mu}{k_BT})}. \tag{2.280}$$

Here we have used the property

$$\partial_z I_n^{\mp}(z) = \pm(n-1) I_{n-1}^{\mp}(z), \tag{2.281}$$

which follows directly from the series expansion (2.274). For large T, we obtain from Eqs. (2.275) and (2.277) the limit

$$T\partial_T \frac{\mu}{k_B T} \xrightarrow[T\to\infty]{} -\frac{3}{2}. \tag{2.282}$$

Relation (2.270) can also be obtained from the general thermodynamic calculation

$$E - \mu N = -Z_G^{-1}\frac{\partial Z_G}{\partial\beta} = \frac{\partial}{\partial\beta}\beta F_G, \tag{2.283}$$

which follows directly from (2.251) by differentiating with respect to $\beta = 1/k_B T$.

The grand-canonical free energy is from (2.268) with (2.262), (2.266), (2.272), and (2.273):

$$\begin{aligned} F_G(T,\mu,V) = -pV &= -g\frac{V}{\lambda^3(T)} k_B T \frac{2}{3}\frac{2}{\sqrt{\pi}} I_{5/2}^{\mp}\left(\frac{\mu}{k_B T}\right) \\ &= -N(T,\mu)\, k_B T\, \frac{2}{3}\frac{I_{5/2}^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}. \end{aligned} \tag{2.284}$$

For large T where $\alpha \to -\infty$, the limiting formula (2.277) shows that F_G has the correct Dulong-Petit behavior $-Nk_BT$ implying the ideal-gas law $pV = Nk_BT$.

Due to relation (2.270), the energy is

$$E = N(T,\mu)\, k_B T\, \frac{I_{5/2}^{\mp}(\frac{\mu}{k_B T})}{I_{3/2}^{\mp}(\frac{\mu}{k_B T})}. \tag{2.285}$$

For large temperatures, this has the correct Dulong-Petit limit of free particles $3Nk_BT/2$.

By differentiating the first line in Eq. (2.284) with respect to μ and using the relation (2.281), we see that this equality ensures the thermodynamic relation $N = -\partial F_G/\partial\mu$.

According to Eq. (1.292), the entropy S is obtained from the negative derivative of (2.284) with respect to T. This yields

$$S = k_B g\frac{V}{\lambda^3(T)}(k_B T)^{3/2}\frac{2}{\sqrt{\pi}} I_S^{\mp}\left(\frac{\mu}{k_B T}\right) = k_B N(T,\mu)\frac{2}{3}\frac{I_S^{\mp}\left(\frac{\mu}{k_B T}\right)}{I_{3/2}^{\mp}\left(\frac{\mu}{k_B T}\right)}, \tag{2.286}$$

where

$$I_S^{\mp}(\alpha) \equiv \frac{5}{2} I_{5/2}^{\mp}(\alpha) - \alpha I_{5/2}^{\mp\prime}(\alpha) = \frac{5}{2} I_{5/2}^{\mp}(\alpha) \mp \frac{3}{2}\alpha I_{3/2}^{\mp}(\alpha). \tag{2.287}$$

This agrees with the general thermodynamic relation

$$F_G(T,\mu) = E(T,\mu) - \mu N(T,\mu) - TS(T,\mu). \tag{2.288}$$

Adiabatic processes are defined by the condition S/N = const., which implies the relation V/k_BT=const. From (2.271) we see that then

$$VT^{3/2}\big|_{\rm adiab} = \text{const.} \tag{2.289}$$

Together with Eq. (2.285), this also amounts to

$$pV^{5/3}\big|_{\rm adiab} = \text{const.} \tag{2.290}$$

The specific heat at constant volume and particle number is found from the entropy forming $C_V = T\partial_T S$ using (2.280). The result is

$$C_V = k_B N\,\frac{1}{2}\left[5\frac{I^{\mp}_{5/2}(\alpha)}{I^{\mp}_{3/2}(\alpha)} \mp 9\frac{I^{\mp}_{3/2}(\alpha)}{I^{\mp}_{1/2}(\alpha)}\right], \qquad \alpha = \frac{\mu}{k_BT}. \tag{2.291}$$

For large T, we use again (2.277) to show that this goes against a constant

$$C_V \xrightarrow[T\to\infty]{} k_B N\frac{3}{2}, \tag{2.292}$$

which complies with the classical rule of Dulong and Petit.

2.14.2 The Degenerate Fermi Gas Near $T = 0$

Consider the Fermi gas close to zero temperature which is called the *degenerate limit*. Then the occupation number (2.266) reduces to

$$\begin{aligned} n_\varepsilon &= \left\{\begin{matrix} 1 \\ 0 \end{matrix}\right. \text{ for } \begin{matrix} \varepsilon < \mu \\ \varepsilon > \mu \end{matrix} \\ &= \Theta(\varepsilon - \mu). \end{aligned} \tag{2.293}$$

All states with energy lower than μ are filled, all higher states are empty. The chemical potential μ at zero temperature is called Fermi energy $\varepsilon_{\rm F}$:

$$\mu\big|_{T=0} \equiv \varepsilon_{\rm F}. \tag{2.294}$$

The Fermi energy for a given particle number N is found from (2.262), (2.265), and (2.293):

$$N = gV\int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon = gV\int_0^{\varepsilon_{\rm F}} d\varepsilon N_\varepsilon = gV\frac{\sqrt{2}M^{3/2}\varepsilon_{\rm F}^{3/2}}{3\pi^2\hbar^3} = gV\frac{p_{\rm F}^3}{6\pi^2\hbar^3}, \tag{2.295}$$

where

$$p_{\rm F} = \sqrt{2M\varepsilon_{\rm F}} \tag{2.296}$$

is the Fermi momentum associated with the Fermi energy. Equation (2.295) is solved for $\varepsilon_{\rm F}$ by

$$\varepsilon_{\rm F} = \left(\frac{6\pi^2}{g}\right)^{2/3}\left(\frac{N}{V}\right)^{2/3}\frac{\hbar^2}{2M}, \tag{2.297}$$

and for the Fermi momentum by

$$p_{\mathrm{F}} = \left(\frac{6\pi^2}{g}\right)^{1/3} \left(\frac{N}{V}\right)^{1/3} \hbar. \tag{2.298}$$

Note that in terms of the particle number N, the density of states per unit energy interval and volume (2.262) can be written as

$$N_\varepsilon \equiv \frac{3}{2}\frac{N}{V}\frac{1}{\varepsilon_{\mathrm{F}}}\sqrt{\frac{\varepsilon}{\varepsilon_{\mathrm{F}}}}. \tag{2.299}$$

As the gas is heated slightly, the degeneracy in the particle distribution function in Eq. (2.293) softens. The degree to which this happens is governed by the size of the ratio $kT/\varepsilon_{\mathrm{F}}$. It is useful to define a characteristic temperature, the so-called Fermi Temperature

$$T_{\mathrm{F}} \equiv \frac{\varepsilon_{\mathrm{F}}}{k_B} = \frac{1}{k_B}\frac{{p_{\mathrm{F}}}^2}{2M}. \tag{2.300}$$

For electrons in a metal, p_{F} is of the order of $\hbar/1\text{Å}$, Inserting $M = m_e = 9.109558 \times 10^{-28}$ g, further $k_B = 1.380622 \times 10^{-16}$ erg/K and $\hbar = 6.0545919 \times 10^{-27}$ erg sec, we see that T_{F} has the order of magnitude

$$T_{\mathrm{F}} \approx 44\,000\text{K}. \tag{2.301}$$

Hence, even far above room temperatures the relation

$$T/T_{\mathrm{F}} \ll 1 \tag{2.302}$$

is quite well fulfilled and can be used as an expansion parameter in evaluating the thermodynamic properties of the electron gas at nonzero temperature.

Let us now calculate the corrections at small $T \neq 0$. From (2.271) we have the particle number

$$N = N(T,\mu) \equiv g\frac{V}{\lambda^3(T)}\frac{2}{\sqrt{\pi}} I^+_{3/2}\left(\frac{\mu}{k_BT}\right), \tag{2.303}$$

from (2.284) the grand-canonical free energy

$$\begin{aligned} F_G(T,\mu,V) = -pV &= -g\frac{V}{\lambda^3(T)}k_BT\frac{2}{3}\frac{2}{\sqrt{\pi}}\, I^+_{5/2}\left(\frac{\mu}{k_BT}\right) \\ &= -N(T,\mu)\,k_BT\,\frac{2}{3}\frac{I^+_{5/2}(\frac{\mu}{k_BT})}{I^+_{3/2}(\frac{\mu}{k_BT})}, \end{aligned} \tag{2.304}$$

and from (2.285) the energy

$$E = N(T,\mu)\,k_BT\,\frac{I^+_{5/2}(\frac{\mu}{k_BT})}{I^+_{3/2}(\frac{\mu}{k_BT})}. \tag{2.305}$$

Eliminating the particle number in favor of the Fermi energy with the help of Eq. (2.295), we obtain for the temperature dependence of the chemical potential the equation

$$1=\left(\frac{k_BT}{\varepsilon_{\rm F}}\right)^{3/2}\frac{3}{2}I^+_{3/2}\left(\frac{\mu}{k_BT}\right). \tag{2.306}$$

For $T\to 0$, the chemical potential μ approaches the Fermi energy $\varepsilon_{\rm F}$, so that small temperatures correspond to large $\alpha=\mu/k_BT$. In the regime $T/T_{\rm F}\ll 1$ one may derive expansions in powers of $T/T_{\rm F}$. These expansions will be asymptotic, diverging even for infinitesimally small T. They can nevertheless be used for calculating these functions for sufficiently small T. For larger T they need resummations. Setting

$$z-\alpha\equiv x \tag{2.307}$$

and writing

$$\begin{aligned} I^+_n(\alpha) &= \int_{-\alpha}^{\infty}dx\frac{(\alpha+x)^{n-1}}{e^x+1}\\ &= \int_0^{\alpha}dx\frac{(\alpha-x)^{n-1}}{e^{-x}+1}+\int_0^{\infty}dx\frac{(\alpha+x)^{n-1}}{e^x+1}. \end{aligned} \tag{2.308}$$

In the first integral we substitute

$$\frac{1}{e^{-x}+1}=1-\frac{1}{e^x+1} \tag{2.309}$$

and find the expression

$$I^+_n(\alpha)=\int_0^{\alpha}dx\,x^{n-1}+\int_0^{\infty}dx\frac{(\alpha+x)^{n-1}-(\alpha-x)^{n-1}}{e^x+1}+\int_{\alpha}^{\infty}dx\frac{(\alpha-x)^{n-1}}{e^x+1}. \tag{2.310}$$

In the limit $\alpha\to\infty$, only the first term survives, whereas the last term is exponentially small, so that it can be ignored in a power series expansion. The second term is expanded as

$$2\sum_{k=\rm odd}^{\infty}\binom{n-1}{k}\alpha^{n-1-k}\int_0^{\infty}dx\frac{x^k}{e^x+1}=2\sum_{k=\rm odd}\frac{(n-1)!}{(n-1-k)!}\alpha^{n-1-k}(1-2^{-k})\zeta(k+1). \tag{2.311}$$

At even positive and odd negative integer arguments, the zeta function is related to the Bernoulli numbers by[4]

$$\zeta(1-2n)=-\frac{B_{2n}}{2n},\qquad \zeta(2n)=\frac{(2\pi)^{2n}}{2(2n)!}|B_{2n}|. \tag{2.312}$$

The two equations go over into each other via the identity

$$\zeta(x)=2^x\pi^{x-1}\sin(\pi x/2)\Gamma(1-x)\zeta(1-x), \tag{2.313}$$

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[4] These and the subsequent formulas are found in I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formulas 9.542 and 9.535.

which can also be written as

$$\zeta(x) = 2^{x-1}\pi^x \zeta(1-x)/\Gamma(x)\cos\frac{x\pi}{2}. \tag{2.314}$$

The lowest values of $\zeta(x)$ occurring in the expansions are[5]

$$\zeta(2) = \frac{\pi^2}{6}, \quad \zeta(4) = \frac{\pi^4}{90}, \tag{2.315}$$

so that the expansion of $I_n(\alpha)$ starts out like

$$I_n(\alpha) = \frac{1}{n}\alpha^n + 2(n-1)\frac{1}{2}\zeta(2)\alpha^{n-2} + 2(n-1)(n-2)(n-3)\frac{7}{8}\zeta(4)\alpha^{n-4} + \ldots\,. \tag{2.316}$$

Inserting this with $n = 3/2$ into Eq. (2.306), we find

$$1 = \left(\frac{k_BT}{\varepsilon_{\rm F}}\right)^{3/2}\frac{3}{2}\left[\frac{2}{3}\left(\frac{\mu}{k_BT}\right)^{3/2} + \frac{\pi^2}{12}\left(\frac{\mu}{k_BT}\right)^{-1/2} + \frac{7\pi^4}{3\cdot 320} + \left(\frac{\mu}{k_BT}\right)^{-5/2}\ldots\right], \tag{2.317}$$

or

$$\mu = \varepsilon_{\rm F}\left[1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\varepsilon_{\rm F}}\right)^2 + \frac{7\pi^4}{720}\left(\frac{k_BT}{\varepsilon_{\rm F}}\right)^4 + \ldots\right], \tag{2.318}$$

In the grand-canonical free energy F_G which contains $I^+_{3/2}$ we obtain the expansion

$$F_G(T,\mu,V) = F_G(0,\mu,V)\left[1 + \frac{5\pi^2}{8}\left(\frac{k_BT}{\mu}\right)^2 - \frac{7\pi^4}{384}\left(\frac{k_BT}{\mu}\right)^4 + \ldots\right], \tag{2.319}$$

where

$$F_G(0,\mu,V) \equiv -\frac{2}{5}gV\frac{\sqrt{2}M^{3/2}}{3\pi^2\hbar^3}\mu^{5/2}.$$

Indeed, from (2.304) we find for $T \to 0$:

$$F_G(0,\varepsilon_{\rm F},V) = -\frac{2}{5}N\mu. \tag{2.320}$$

By differentiating F_G with respect to the temperature at fixed μ, we obtain the low-temperature behavior of the entropy

$$S = k_B\frac{\pi^2}{2}\frac{k_BT}{\varepsilon_{\rm F}}\frac{N}{V} + \ldots\,. \tag{2.321}$$

From this we find a specific heat

$$\begin{aligned} C_V &= T\left.\frac{\partial S}{\partial T}\right|_{V,N} = \frac{\pi^2}{2}\frac{k_BT}{\varepsilon_{\rm F}}N \\ &= \frac{g}{2}\frac{Mp_{\rm F}}{3}Nk_BT. \end{aligned} \tag{2.322}$$

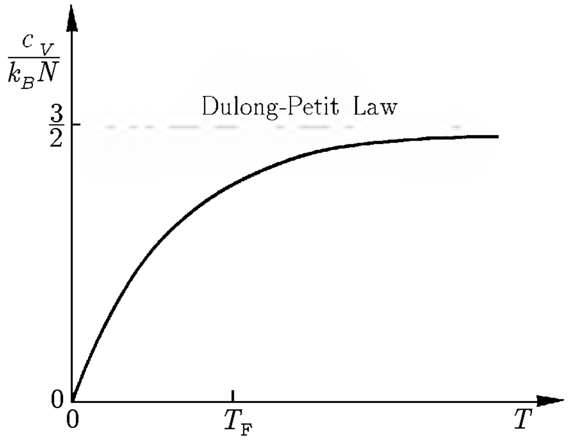

FIGURE 2.3 Temperature behavior of specific heat of a free Fermi gas.

This grows linearly with increasing temperature (see Fig. 2.3 for the full temperature behavior). The linear behavior is due to the progressive softening near the surface of the Fermi distribution which makes more and more electrons thermally excitable. It is detected experimentally in metals at low temperature where the contribution of lattice vibrations freezes out as $(T/T_D)^3$. Here T_D is the Debye temperature which characterizes the elastic stiffness of the crystal and ranges from $T_D \approx 90$K in soft metals like lead over $T_D \approx 389$K for aluminum to $T_D \approx 1890$K for diamond. The experimental size of the slope is usually larger than the free electron gas value in (2.322). This can be explained mainly by the interactions with the lattice which result in a large effective mass $M_{\rm eff} > M$.

Note that the quantity $F_G(0,\mu,V)$ is temperature-dependent via the chemical potential μ. Inserting (2.318) into (2.319) we find the complete T-dependence

$$F_G(T,\mu,V) = F_G(0,\varepsilon_{\rm F},V)\left[1+\frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_{\rm F}}\right)^2 - \frac{\pi^4}{16}\left(\frac{k_BT}{\varepsilon_{\rm F}}\right)^4 + \ldots\right]. \tag{2.323}$$

with $F_G(0,\varepsilon_{\rm F},V)$ given by Eq. (2.320) at $\mu=\varepsilon_{\rm F}$.

Recalling the relation (2.270), this equation supplies us with the low-temperature behavior of the internal energy:

$$E = \frac{3}{5}N\varepsilon_{\rm F}\left[1+\frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 - \frac{\pi^4}{16}\left(\frac{k_BT}{\varepsilon_F}\right)^4 + \ldots\right]. \tag{2.324}$$

The first term is the energy of the zero-temperature Fermi sphere. Using the relation $C_V = \partial E/\partial T$, the second term yields once more the leading $T\to 0$ behavior (2.322) of the specific heat.

---

[5] Other often-needed values are $\zeta(0) = -1/2$, $\zeta'(0) = -\log(2\pi)/2$, $\zeta(-2n) = 0$, $\zeta(3) \approx 1.202057$, $\zeta(5) \approx 1.036928, \ldots$.

This behavior of the specific heat can be observed in metals where the conduction electrons behave like a free electron gas. Due to *Bloch's theorem*, a single electron in a perfect lattice behave just like a free particle. For many electrons, this is still approximately true, if the mass of the electrons is replaced by an effective mass.

Another important macroscopic system where (2.322) can be observed is a liquid consisting of the fermionic isotope ^{3}He. There are two electron spins and an odd number of nucleon spins which make this atom a fermion. The atoms interact strongly in the liquid, but it turns out that these interactions produce a screening effect after which the system may be considered approximately as an almost-free gas of quasiparticles which behave like free fermions whose mass is about 8 times that of the strongly interacting atoms.

2.14.3 Degenerate Bose Gas Near $T = 0$

For bosons, the low temperature discussion is quite different. As we can see from Eq. (2.265), the particle density remains positive for all $\varepsilon \in (0, \infty)$ only if the chemical potential μ is negative. A positive μ would also cause a divergence in the integrals (2.271), (2.273). At large temperatures, the chemical potential has a large negative value, which moves closer to zero as the temperature decreases (see Fig. 2.4, compare also Fig. 2.1). The chemical potential vanishes at a critical temperature T_c. From Eqs. (2.271), and (2.275), this is determined by the equation

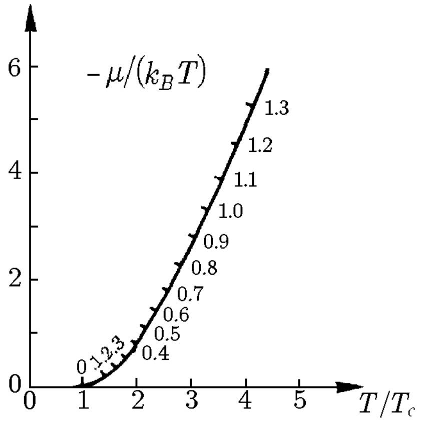

FIGURE 2.4 Temperature behavior of the chemical potential of a free Bose gas.

$$\begin{aligned} \frac{N}{V} &= g\int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon \\ &= g\frac{V}{\lambda^3(T)}\frac{2}{\sqrt{\pi}}I^-_{3/3}\left(\frac{\mu}{k_BT}\right), \end{aligned} \tag{2.325}$$

at $\mu = 0$, where it yields, via Eq. (2.275), the particle density

$$\frac{N}{V} = g\frac{V}{\lambda^3(T)}\zeta(3/2). \tag{2.326}$$

Thus the critical temperature T_c satisfies the equation

$$T_c = [g\zeta(3/2)]^{-2/3}\left(\frac{N}{V}\right)^{2/3}\frac{2\pi\hbar^2}{k_BM}, \tag{2.327}$$

with $\zeta(3/2) = 2.61238\ldots$. Using this we rewirte Eq. (2.271) in the simpler form

$$1 = \left(\frac{T}{T_c}\right)^{3/2}\frac{I_{3/2}(\alpha)}{I_{3/2}(0)}, \qquad \alpha = \frac{\mu}{k_BT}. \tag{2.328}$$

For α between 0 and 1, this equation yields $T/T_c > 1$, while Eq. (2.291) gives us the associated specific heat. The result is deferred to Fig. 2.6, after we have understood what happens for small temperatures $T < T_c$ where (2.271) has no solution. Here we only note that since $I_{1/2}(0) = \infty$, the specific heat (2.291) has a peak at T_c of height

$$C_V^{\max} = k_BN\,\frac{5}{2}\frac{I_{5/2}(0)}{I_{3/2}(0)} = k_BN\,\frac{5}{2}\frac{\Gamma(5/2)\zeta(5/2)}{\Gamma(3/2)\zeta(3/2)} \approx k_BN\,1.92567. \tag{2.329}$$

From Eq. (2.327) we see that the phase transition takes place when the average distance beteen atoms becomes smaller than the De Broglie wavelength of thermal motion (2.272), which for helium is rougly equal to 5.64Å.[6]

For $T < T_c$, Eq. (2.271) has no solution even though the physical system can be cooled further. The apparent contradiction has its origin in a failure of the replacement (2.259) for $T < T_c$. The reason is that the state with $\mathbf{p} = 0$ has no energy and fails to be counted in the energy integral over all states in Eq. (2.271). To avoid this we have to write more properly

$$N = N_{\mathbf{p}=\mathbf{0}} + N_{\mathbf{p}\neq\mathbf{0}} \equiv N_s + gV\int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon|_{\mu=0}. \tag{2.330}$$

where N_s is the number of Bose particles at zero momentum and energy. Below T_c, a finite fraction of all particles N_s/N accumulates in this single degenerate state. It can be calculated from the modified Eq. (2.325):

$$\begin{aligned} N - N_s &= Vg\int_0^\infty d\varepsilon N_\varepsilon n_\varepsilon|_{\mu=0} \\ &= g\frac{V}{\lambda^3(T)}\frac{2}{\sqrt{\pi}}I^-_{3/2}(0) = N\left(\frac{T}{T_c}\right)^{3/2}. \end{aligned} \tag{2.331}$$

Thus we find that the number of degenerate bosons has the temperature behavior

$$N_s = N\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right], \tag{2.332}$$

which is plotted in Fig. 2.6.

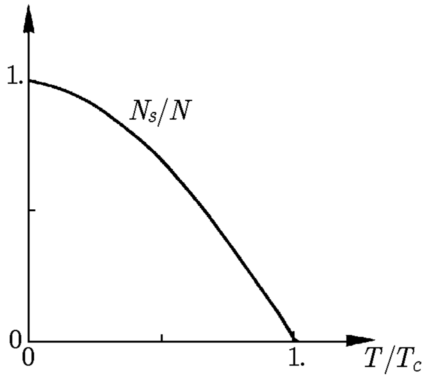

FIGURE 2.5 Temperature behavior of fraction of degenerate bosons in the zero-momentum state of a free Bose gas.

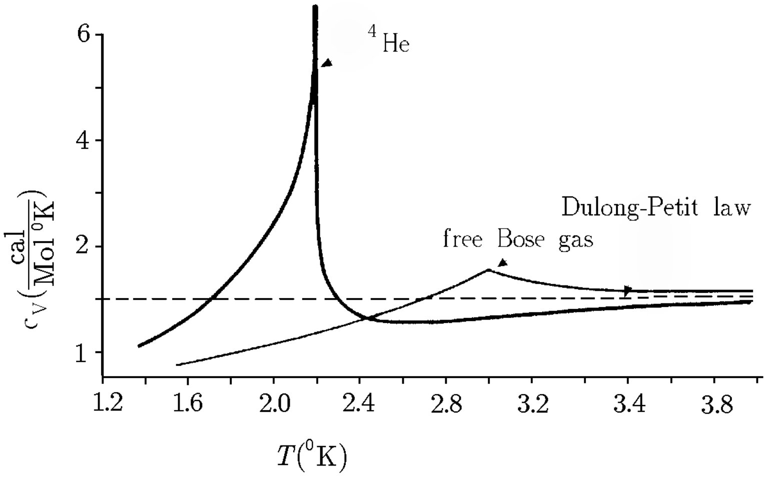

FIGURE 2.6 Temperature behavior of the specific heat of a free boson gas. For comparison we show the specific heat of the strongly interacting Bose liquid ^{4}He, scaled down by a factor 2 to match the Dulong-Petit limit of the free Bose gas.

The phenomenon of a macroscopic accumulation of particles in a single state is called *Bose condensation* and plays a central role in the understanding of the phenomenon of *superfluidity* in liquid helium consisting of the bosonic atoms ^{4}He.

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[6] See p. 256 of the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I World Scientific, Singapore, 1989.

In fact, the temperature T_c calculated from Eq. (2.327) is $T_c \sim 3.1\text{K}$ which is roughly of the same order as the experimental value[7]

$$T_c^{\text{exp}} \equiv 2.18\text{K}. \tag{2.333}$$

The discrepancy is due to the strong interactions between the ^{4}He atoms in the liquid state which have all been neglected in deriving Eq. (2.333).

There exists a phenomenological two-fluid description of superfluidity in which the condensate of the $\mathbf{p} = \mathbf{0}$ bosons is identified with the *superfluid component* of the liquid. This is the reason why we have used the subscript s in (2.331). The complementary piece

$$N_n = N - N_s \tag{2.334}$$

is usually referred to as the *normal component* of the superfluid.

For $T < T_c$, the energy of the normal liquid is equal to the total energy. Using Eq. (2.285) with $\mu = 0$ we find

$$\begin{aligned} E_n &= E = g\frac{V}{\lambda^3(T)}\frac{2}{\sqrt{\pi}}k_BTI_{5/2}^-(0) = \frac{\Gamma(5/2)\zeta(5/2)}{\Gamma(3/2)\zeta(3/2)}Nk_BT\left(\frac{T}{T_c}\right)^{3/2} \\ &\approx 0.7703\,Nk_BT\left(\frac{T}{T_c}\right)^{3/2}, \end{aligned} \tag{2.335}$$

having inserted $\zeta(5/2) \approx 1.341$ and $\Gamma(5/2) = 3\sqrt{\pi}/4$. From this energy we find the specific heat below T_c:

$$\begin{aligned} C_V &= T\frac{\partial S}{\partial T}\bigg|_{V,N} = \frac{\partial E}{\partial T}\bigg|_{V,N} \\ &= \frac{5}{2}\frac{E}{T} \propto T^{3/2}. \end{aligned} \tag{2.336}$$

Integrating this with respect to the temperature gives the entropy

$$S = \frac{5}{3}\frac{E}{T}, \tag{2.337}$$

and the free energy $F = E - TS$ takes the simple form

$$F = -\frac{2}{3}E. \tag{2.338}$$

This is consistent with the general result Eq. (2.269) since for $\mu = 0$, the grand canonical free energy F_G coincides with the free energy F [recall the Euler relation (1.301)].

The special role of the Bose condensate lies in the fact that it provides the system with a particle reservoir, with the relation Eq. (2.271) being replaced by Eq. (2.325) and Eq. (2.331).

---

[7] The density is $\rho \approx 0.145$ g/cm^3, i.e., the volume per atom is $V/N \approx 46.2\text{Å}^3$, and $M_{^4\text{He}} \approx 4m_{\text{p}} \approx 4 \times 1.6762 \times 10^{-24}$g.

According to Eq. (2.336), the specific heat increases with a power $T^{3/2}$:

$$C_V = \frac{\partial E}{\partial T} = k_B N \frac{5}{2}\frac{\Gamma(5/2)\zeta(5/2)}{\Gamma(3/2)\zeta(3/2)} \left(\frac{T}{T_c}\right)^{3/2} \approx k_B N\, 1.92567 \left(\frac{T}{T_c}\right)^{3/2}. \tag{2.339}$$

Comparison with (2.329) shows that at T_c this has the same maximal value at $T = T_c$ as the solution for $T > T_c$.

As T passes T_c, the chemical potential starts growing. To calculate this behavior let us decompose Eq. (2.325) as

$$N = g \frac{V}{\lambda^3(T)} \frac{2}{\sqrt{\pi}} \left[I^-_{3/2}(0) + \Delta I^-_{3/2}\left(\frac{\mu}{k_B T}\right)\right] \tag{2.340}$$

with

$$\Delta I^-_{3/2}(\alpha) \;=\; \int_0^\infty dz\, z^{1/2} \left(\frac{1}{e^{z-\alpha}-1} - \frac{1}{e^z - 1}\right). \tag{2.341}$$

The first term in (2.340) is simply

$$N_n(T) \equiv N \left(\frac{T}{T_c}\right)^{3/2}. \tag{2.342}$$

The second term receives its main contribution from $z \approx 0$, where $\Delta I^-_{3/2}(\alpha)$ can be approximated by

$$\Delta I^-_{3/2}(\alpha) \approx \alpha \int_0^\infty dz \frac{1}{z^{1/2}(z-\alpha)} = -\pi\sqrt{-\alpha}. \tag{2.343}$$

Hence we can write

$$N = N_n(T) \left[1 + \frac{\Delta I^-_{3/2}\left(\frac{\mu}{k_B T}\right)}{I^-_{3/2}(0)} \right], \tag{2.344}$$

or

$$\frac{N_n(T)}{N} - 1 \approx -\frac{\Delta I^-_{3/2}\left(\frac{\mu}{k_B T}\right)}{I^-_{3/2}(0)}. \tag{2.345}$$

This makes $-\mu$ increase for $T \gtrsim T_c$ like

$$-\mu \approx \frac{1}{\pi^2} k_B T_c \, [I^-_{3/2}(0)]^2 \left[\frac{N_n(T)}{N} - 1 \right]^2. \tag{2.346}$$

Using the relation (2.269) we calculate the derivative of the energy with respect to the chemical potential from

$$\left.\frac{\partial E}{\partial \mu}\right|_{T,V} = -\frac{3}{2} \left.\frac{\partial F_G}{\partial \mu}\right|_{T,V}. \tag{2.347}$$

This allows us to find the internal energy slightly above the critical temperature T_c, where $-\mu$ is small, as

$$\begin{aligned} E &\approx E_n + \frac{3}{2}N\mu. \\ &= E_n - \frac{3}{2\pi^2}Nk_BT_c\,[I^-_{3/2}(0)]^2\left[\left(\frac{T}{T_c}\right)^{3/2} - 1\right]^2. \end{aligned} \tag{2.348}$$

Forming the derivative with respect to temperature as in (2.336) we see that at T_c the specific heat has a kink. Its slope jumps by

$$\Delta\left(\frac{\partial C_V}{\partial T}\right) \approx \frac{27}{4\pi^2}[I^-_{3/2}(0)]^2\,N\frac{k_B}{T_c} \equiv 3.6658\,N\frac{k_B}{T_c}, \tag{2.349}$$

the slopes being from (2.335)

$$\left(\frac{\partial C_V}{\partial T}\right) = \frac{5}{2}\frac{3}{2}\frac{I_{5/2}(0)}{I_{3/2}(0)}\frac{Nk_B}{T_c} \approx \frac{5}{2}\frac{3}{2}0.7703\frac{Nk_B}{T_c} \approx 2.8885\frac{Nk_B}{T_c}, \qquad T \le T_c, \tag{2.350}$$

and from (2.348):

$$\left(\frac{\partial C_V}{\partial T}\right) = \left[\frac{5}{2}\frac{3}{2}\frac{I_{5/2}(0)}{I_{3/2}(0)} - \frac{27}{4\pi^2}[I^-_{3/2}(0)]^2\right]\frac{Nk_B}{T_c} \approx -0.7715\frac{Nk_B}{T_c}, \qquad T > T_c. \tag{2.351}$$

Let us compare the behavior of the specific heat of the free Bose gas with the experimental results for the Bose liquid ^{4}He (see Fig. 2.6). The latter also rises like T^3 for small T, but it has a sharp singularity at $T = T_c$. Considering the crudeness of the free gas approximation the similarity of the curves is quite surprising, indicating at least the physical relevance of the above idealized quantum-statistical description.

2.14.4 High Temperatures

At high temperatures, the particles are distributed over a large volume in phase space, so that the occupation numbers of each energy level are very small. As a consequence, the difference between bosons and fermions disappears, and the distribution functions (2.266) become

$$n_\varepsilon \equiv -\frac{\partial}{\partial\mu}F_\varepsilon(T,\mu) \approx e^{(\mu-\varepsilon)/k_BT}, \tag{2.352}$$

for either statistics. The high-temperature limit of the thermodynamic quantities can therefore all be calculated from the fermion expressions. The corresponding limit in the functions $I^\mp_n(\alpha)$ in Eq. (2.273) is $\alpha \to -\infty$, for which we obtain

$$I^\mp_n(\alpha) \xrightarrow[\alpha\to-\infty]{} \int_0^\infty z^n e^{\alpha - z} = n!e^\alpha. \tag{2.353}$$

Inserting this for $n = 1/2$ into (2.299), we find that for a fixed particle number N, the chemical potential has the large-T behavior

$$\frac{\mu}{k_BT} \approx \frac{3}{2}\log\left[\frac{k_BT}{\varepsilon_{\rm F}}\left(\frac{3\sqrt{\pi}}{4}\right)^{2/3}\right]. \tag{2.354}$$

In the same limit, the grand-canonical free energy (2.284) behaves like

$$F_G(T,\mu,V) \approx -N(T,\mu)\,k_BT. \tag{2.355}$$

With the definition of the pressure (1.299), this is the equation of state for the *ideal gas*. Using the relation (2.269), we obtain from this the internal energy at a fixed particle number

$$E \approx \frac{3}{2}N\,k_BT. \tag{2.356}$$

This equation is a manifestation of the *Dulong-Petit law*: Each of the $3N$ degrees of freedom of the system carries an internal energy $k_BT/2$.

The corresponding specific heat per constant unit volume is

$$C_V = N\frac{3}{2}k_B. \tag{2.357}$$

2.15 Temperature Green Functions of Free Particles

As argued in Section 1.7, all properties of a system in thermodynamic equilibrium are calculable by continuing the quantum theory to imaginary times $t = -i\tau$ with real τ. We shall see later that the calculation of small interaction effects to the free-particle results presented in the last section can be done perturbatively. It involves the analytically continued analog of the free-particle propagator (2.235).

In a grand-canonical ensemble, the relevant quantity is the so called *temperature Green function* (or propagator) of free particles:

$$\begin{aligned} G(\mathbf{x},\tau;\mathbf{x}'\tau') &= \frac{\mathrm{Tr}\left[e^{-\hat{H}_G/k_BT}\hat{T}_\tau\left(\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')\right)\right]}{\mathrm{Tr}\left(e^{-\hat{H}_G/k_BT}\right)} \\ &= e^{F_G/k_BT}\mathrm{Tr}\left[e^{-\hat{H}_G/k_BT}\hat{T}_\tau\left(\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')\right)\right], \end{aligned} \tag{2.358}$$

where $\hat{T}_\tau$ is the τ-ordering operator defined in complete analogy to the time-ordering operator $\hat{T}$ in (2.233). The fields $\hat{\psi}(\mathbf{x},\tau), \hat{\psi}^\dagger(\mathbf{x},\tau)$ are defined in analogy to (2.131) and (2.132) via an analytically continued time evolution operator as follows:

$$\hat{\psi}(\mathbf{x},\tau) = e^{\hat{H}_G\tau/\hbar}a_{\mathbf{x}}e^{-\hat{H}_G\tau/\hbar}, \tag{2.359}$$

$$\hat{\psi}^\dagger(\mathbf{x},\tau) = e^{-\hat{H}_G\tau/\hbar}\hat{a}^\dagger_{\mathbf{x}}e^{\hat{H}_G\tau\hbar}. \tag{2.360}$$

These satisfy canonical commutation relations at equal imaginary time analogous to (2.206):

$$\begin{aligned}
[\hat{\psi}(\mathbf{x},\tau),\hat{\psi}(\mathbf{x}',\tau)]_{\mp} &= 0,\\
[\hat{\psi}^{\dagger}(\mathbf{x},\tau),\hat{\psi}^{\dagger}(\mathbf{x}',\tau)]_{\mp} &= 0,\\
[\hat{\psi}(\mathbf{x},\tau),\hat{\psi}^{\dagger}(\mathbf{x}',\tau)]_{\mp} &= \delta^{(3)}(\mathbf{x}-\mathbf{x}'),
\end{aligned} \tag{2.361}$$

The time evolution of these field operators is goverend by the grand-canonical Hamiltonian

$$\hat{H}_G = \hat{H} - \mu\hat{N}. \tag{2.362}$$

Note that while $\psi^{\dagger}_{\mathbf{p}}$ is the Hermitian conjugate of $\psi_{\mathbf{p}}$ at $\tau = 0$, this is no longer true for $\tau \neq 0$. The advantages of using these non-Hermitian fields will become apparent later when we discuss perturbation theory.

When it comes to calculating physical observables, only Green functions with an imaginary time variable in the interval

$$\tau \in (0, \hbar/k_BT), \tag{2.363}$$

will be needed. In the present discussion, however, we consider the behavior for all τ.

Differentiating (2.359) and (2.360) with respect to τ, we obtain the Heisenberg equations

$$\partial_\tau\hat{\psi}(\mathbf{x},\tau) = [\hat{H}_G,\hat{\psi}(\mathbf{x},\tau)], \partial_\tau\hat{\psi}^{\dagger}(\mathbf{x},\tau) = -[\hat{H}_G,\hat{\psi}(\mathbf{x},\tau)]. \tag{2.364}$$

Using the canonical field commutation relations (2.361), the fields $\hat{\psi}(\mathbf{x},\tau)$ and $\hat{\psi}^{\dagger}(\mathbf{x},\tau)$ are seen to satisfy the analytically continued Schrödinger equations

$$\left(-\hbar\partial_\tau + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}^2 + \mu\right)\hat{\psi}(\mathbf{x},\tau) = 0, \tag{2.365}$$

$$\hat{\psi}^{\dagger}(\mathbf{x},\tau)\left(\hbar\overleftarrow{\partial}_\tau + \frac{\hbar^2}{2M}\overleftarrow{\partial}_{\mathbf{x}}^{\,2} + \mu\right) = 0. \tag{2.366}$$

The plane-wave solutions of these equations are the analytically-continued versions of the plane-wave solutions (2.207), with particle energies counted from the chemical potential μ rather than zero. The canonical field operators solving (2.365) and (2.366) have expansions (2.216). Explicitly:

$$\begin{aligned}
\hat{\psi}(\mathbf{x},\tau) &= \int \bar{d}^3p\, e^{i\mathbf{px}/\hbar-\xi(\mathbf{p})\tau/\hbar}\hat{a}_{\mathbf{p}},\\
\hat{\psi}^{\dagger}(\mathbf{x},\tau) &= \int \bar{d}^3p\, e^{-i\mathbf{px}/\hbar+\xi(\mathbf{p})\tau/\hbar}\hat{a}^{\dagger}_{\mathbf{p}}
\end{aligned} \tag{2.367}$$

Inserting these into (2.358), we now calculate the Green function for $\tau > \tau'$

$$\begin{aligned}
G(\mathbf{x},\tau;\mathbf{x}',\tau') &= G(\mathbf{x}-\mathbf{x}',\tau-\tau')\\
&= e^{F_G/k_BT}\mathrm{Tr}\left[e^{-\hat{H}_G/k_BT}\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^{\dagger}(\mathbf{x}',\tau')\right]\\
&= e^{F_G/k_BT}\int \bar{d}^3p\int \bar{d}^3p'\,\mathrm{Tr}\,(e^{-\hat{H}_G/k_BT}\hat{a}_{\mathbf{p}}\hat{a}^{\dagger}_{\mathbf{p}'})e^{i[\mathbf{px}-\mathbf{p}'\mathbf{x}']/\hbar-i[\xi(\mathbf{p})\tau-\xi(\mathbf{p}')\tau']/\hbar}.
\end{aligned} \tag{2.368}$$

Now we observe that

$$e^{F_G/kT}\mathrm{Tr}\left(e^{-\hat{H}_G/k_BT}\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}'}\right)=\frac{\mathrm{Tr}\left(e^{-\hat{H}_G/k_BT}\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}'}\right)}{\mathrm{Tr}\left(e^{-\hat{H}_G/k_BT}\right)}$$

is simply the average particle number of Eq. (2.266) for the energy $\xi(\mathbf{p})$:

$$n_{\xi(\mathbf{p})}=\frac{1}{e^{\xi(\mathbf{p})/k_BT}\mp 1}, \tag{2.369}$$

apart from a Dirac δ-function in the momenta $\delta^{(3)}(\mathbf{p}-\mathbf{p}')$. Hence we find for $\tau>0$:

$$G(\mathbf{x},\tau)\equiv\int d^3p\, e^{i\mathbf{px}/\hbar-\xi(\mathbf{p})\tau/\hbar}(1\pm n_{\xi(\mathbf{p})}). \tag{2.370}$$

For $\tau<0$, the operator order is reversed, and we obtain directly

$$G(\mathbf{x},\tau)\equiv\pm\int d^3p\, e^{i\mathbf{px}/\hbar-\xi(\mathbf{p})\tau/\hbar}n_{\xi(\mathbf{p})}. \tag{2.371}$$

From these expressions we can derive an important property of the temperature Green function. Using the identity

$$e^{\xi/k_BT}n_\xi=1\pm n_\xi, \tag{2.372}$$

we see that $G(\mathbf{x},\tau)$ satisfies the relation

$$G(\mathbf{x},\tau)=\pm G(\mathbf{x},\tau+\frac{\hbar}{k_BT}),\qquad \tau\in(-\frac{\hbar}{k_BT},\frac{\hbar}{k_BT}], \tag{2.373}$$

in particular $G(\mathbf{x},0)=\pm G(\mathbf{x},\hbar/k_BT)$. As a consequence, $G(\mathbf{x},\tau)$ has a Fourier transform

$$G(\mathbf{x},\tau)=\frac{k_BT}{\hbar}\sum_{\omega_m}e^{-i\omega_m\tau}G(\mathbf{x},\omega_m) \tag{2.374}$$

with the frequencies

$$\omega_m\equiv\frac{2\pi k_BT}{\hbar}m, \tag{2.375}$$

where m runs through all integer values $m=0,\pm1,\pm2,\ldots$ for bosons and through all half-integer values $m=\pm1/2,\pm3/2,\ldots$ for fermions. These are known as *Matsubara frequencies*.

The Fourier components are given by the integrals

$$G(\mathbf{x},\omega_m)=\int_0^{\hbar/k_BT}d\tau\, e^{i\omega_m\tau}G(\mathbf{x},\tau). \tag{2.376}$$

The full Fourier representation in space and imaginary time reads

$$G(\mathbf{x},\tau)=\frac{k_BT}{\hbar}\sum_{\omega_m}\int d^3p\, e^{-i\omega_m\tau+i\mathbf{px}/\hbar}G(\mathbf{p},\omega_m) \tag{2.377}$$

with the components

$$\begin{aligned} G(\mathbf{p},\omega_m) &= \int d^3x \int_0^{\hbar/k_BT} d\tau\, e^{i\omega_m\tau - i\mathbf{p}\mathbf{x}/\hbar} G(\mathbf{x},\tau) \\ &= \frac{\hbar}{i\hbar\omega_m - \xi(\mathbf{p})}(1 \pm n_{\xi(\mathbf{p})}) \left\{ e^{[i\hbar\omega_m - \xi(\mathbf{p})]/k_BT} - 1 \right\}. \end{aligned} \tag{2.378}$$

Inserting (2.369) and the explicit form of the Matsubara frequencies (2.375), we obtain

$$G(\mathbf{p},\omega_m) = -\frac{\hbar}{i\hbar\omega_m - \xi(\mathbf{p})}. \tag{2.379}$$

Due to a marvelous cancellation, this has become very simple. In fact, the result can be obtained from the Fourier transform (2.250) of the quantum field theoretic Green function $G(\mathbf{p}, E)$ in two steps: First we continue (2.250) analytically in the energy E to the imaginary off-shell values $E = i\hbar\omega_m$, and second we shift the single-particle energy from $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2M$ to $\xi(\mathbf{p}) = \varepsilon(\mathbf{p}) - \mu$, this being a trivial consequence of the use of $\hat{H}_G = \hat{H} - \mu\hat{N}$ instead of $\hat{H}$.

As a cross check, let us calculate $G(\mathbf{x}, \tau)$ for a very small negative $\tau = -\eta$ from the Fourier representation (2.377) with the components (2.379) for bosons:

$$G(\mathbf{x}, -\eta) = -\int d^3p\, e^{i\mathbf{p}\mathbf{x}/\hbar}\, \frac{k_BT}{\hbar} \sum_{\omega_m} e^{i\omega_m\eta} \frac{\hbar}{-i\omega_m + \xi(\mathbf{p})}. \tag{2.380}$$

The phase factor $e^{i\omega_m\eta}$ is necessary to ensure convergence of the otherwise logarithmically divergent sums. The sum can be performed by changing it into a contour integral

$$-k_BT \sum_{\omega_m} e^{i\omega_m\eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \mp \frac{k_BT}{2\pi i} \int_C dz \frac{e^{\eta z}}{e^{z/k_BT} \mp 1} \frac{1}{z - \xi}. \tag{2.381}$$

The contour of integration C encircles the imaginary z-axis in the positive sense, thereby enclosing all integer or half-integer valued poles at $z = i\omega_m$ (see Fig. 2.7). The upper signs on the right-hand side of (2.381) holds for bosons, the lower for fermions.

We now close the two branches of the contour C by two semicircles Γ_l and Γ_r at infinity. Both contribute nothing since the right-semicircle is suppressed by an exponential factor e^{-z/k_BT}, the left-hand by a factor $e^{\eta z}$. The two closed contours are now shrunk to zero. There is a pole only on the right-hand side, at $z = \xi$ which contributes, by Cauchy's residue theorem,

$$\mp k_BT \sum_{\omega_m} e^{i\omega_m\eta} \frac{1}{i\omega_m - \xi(\mathbf{p})} = \pm \frac{1}{e^{\xi(\mathbf{p})/k_BT} \mp 1} = \pm n_{\xi(\mathbf{p})}, \tag{2.382}$$

which are the Bose and Fermi distribution functions, as implied by Eq. (2.371) for small negative τ.

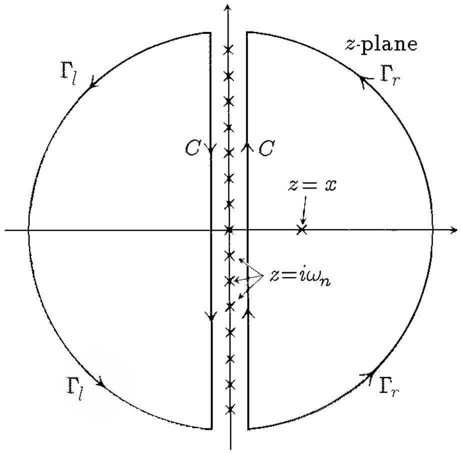

FIGURE 2.7 Contour C in the complex z-plane for evaluating the Matsubara sum (2.382). The semicircles at infinits Γ_l and Γ_r do not contribute. After shrinking the contours, only the pole on the right-hand side contributes via Cauchy's residue theorem.

In the opposite limit $\tau = \eta$, the phase factor in the sum would be $e^{-i\omega_n\eta}$. In this case, the sum is converted into a the contour integral

$$-k_BT\sum_{\omega_n} e^{i\omega_n\eta}\frac{1}{i\omega_n-\xi(\mathbf{p})} = \pm\frac{k_BT}{2\pi i}\int_C dz\,\frac{e^{-\eta z}}{e^{-z/k_BT}\mp 1}\,\frac{1}{z-\xi}, \tag{2.383}$$

from which we would find $1 \pm n_{\xi(\mathbf{p})}$, corresponding to Eq. (2.370) for small positive τ.

While the phase factors $e^{\pm i\omega_m\eta}$ are needed to make the logarithmically-divergent sums converge, they become superfluous if the two sums are combined. Indeed, adding the two sums yields

$$\begin{aligned}
-k_BT\sum_{\omega_n}\left[e^{i\omega_n\eta}\frac{1}{i\omega_n-\xi}+e^{-i\omega_n\eta}\frac{1}{i\omega_n-\xi}\right] &= -k_BT\sum_{\omega_n}e^{i\omega_n\eta}\left[\frac{1}{i\omega_n-\xi}+\frac{1}{-i\omega_n-\xi}\right]\\
&= \frac{k_BT}{\hbar}\sum_{\omega_m}\frac{2\xi}{\omega_m^2+\xi^2} = 1\pm 2\,n_\xi\\
&= \left\{\begin{array}{c}\coth(\hbar\xi/k_BT)\\ \tanh(\hbar\xi/k_BT)\end{array}\right\} \text{ for } \left\{\begin{array}{c}\text{bosons}\\ \text{fermions}\end{array}\right\}.
\end{aligned} \tag{2.384}$$

The right-hand side is the thrermal expecationn value of $\hat{a}_{\mathbf{p}}\hat{a}^{\dagger}_{\mathbf{p}} + \hat{a}^{\dagger}_{\mathbf{p}}\hat{a}_{\mathbf{p}}$.

2.16 Calculating the Matsubara Sum via Poissons Formula

There exists another way of calculating the Matsubara sum in the finite-temperature propagator (2.377). At very low temperature, the Matsubara frequencies $\omega_m =$

$2m\pi k_BT/\hbar$ or $\omega_m = (2m+1)\pi k_BT/\hbar$ move infinitely close to each other, so that the sum over ω_m becomes an integral

$$\frac{k_BT}{\hbar}\sum_{n=-\infty}^{\infty} \to \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi} \tag{2.385}$$

for Bose and Fermi fields. The propagator (2.377) becomes therefore, with (2.379),

$$\begin{aligned} G(\mathbf{x},\tau) &= \frac{k_BT}{\hbar}\sum_{m=-\infty}^{\infty}\int \bar{d}^3p e^{-i\omega_m\tau+i\mathbf{p}\mathbf{x}/\hbar}\frac{i}{\omega_m+i\xi(\mathbf{p})/\hbar} \\ &\to \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\int \bar{d}^3p e^{-i\omega_m\tau+i\mathbf{p}\mathbf{x}/\hbar}\frac{i}{\omega_m+i\xi(\mathbf{p})/\hbar}. \end{aligned} \tag{2.386}$$

The integral over ω_m can be performed trivially with the help of the residue theorem, as in Eq. (2.245), yielding

$$G(\mathbf{p},\tau) = \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}e^{-i\omega_m\tau}\frac{i}{\omega_m+i\xi(\mathbf{p})/\hbar} = \Theta(\tau)e^{-\xi(\mathbf{p})\tau/\hbar}. \tag{2.387}$$

For finite temperatures we make use of Poisson's sum formulas:[8]

$$\sum_{m=-\infty}^{\infty} f(m) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{2\pi i\mu n}f(\mu), \tag{2.388}$$

$$\sum_{m=-\infty}^{\infty} f(m+1/2) = \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} (-)^n e^{2\pi i\mu n}f(\mu). \tag{2.389}$$

A direct application of this formula shows that

$$\frac{k_BT}{\hbar}\sum_{m=-\infty}^{\infty} e^{-i\omega_m\tau}\frac{i}{\omega_m+i\xi(\mathbf{p})/\hbar} = \sum_{n=-\infty}^{\infty}\left\{\begin{matrix}1\\(-1)^n\end{matrix}\right\}\Theta(\tau+n\hbar\beta)e^{-\xi(\mathbf{p})(\tau+n\hbar\beta)/\hbar}. \tag{2.390}$$

Thus the finite-temoperature Green function is obtained from the zero-temperature one by making it periodic or antiperiodic by a simple sum over all periods, with equal or alternating signs. This guarantees the property (2.373).

The sum over n is a geometric series in powers of $e^{-\xi(\mathbf{p})n\hbar\beta}$, which can be performed trivially. For $\tau \in (0,\hbar\beta)$, the Heaviside function forces the sum to run only over positive n, so that we find

$$G(\mathbf{p},\tau) = \sum_{n=0}^{\infty}\left\{\begin{matrix}1\\(-1)^n\end{matrix}\right\}\Theta(\tau+n\hbar\beta)e^{-\xi(\mathbf{p})\tau/\hbar}e^{-n\xi(\mathbf{p})\beta} = \frac{e^{-\xi(\mathbf{p})\tau/\hbar}}{1\mp e^{-\xi(\mathbf{p})\beta}}, \tag{2.391}$$

which can also be rewritten in terms of the Bose and Fermi distribution functions (2.369) as

$$G(\mathbf{p},\tau) = e^{-\xi(\mathbf{p})\tau/\hbar}\left[1\pm n_{\xi(\mathbf{p})}\right]. \tag{2.392}$$

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[8] A proof of this formula is given in Section 2.15 of the textbook H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* World Scientific, Singapore 2002. (http://www.physik.fu-berlin.de/~kleinert/kleiner_re.html#b7).

For a free particles with zero chemical potential where $\xi(\mathbf{p}) = \mathbf{p}^2/2M$, the momentum integral can be done at zero temperature as in Eq. (2.241), and we obtain the imaginary-time version of the Schrödinger propagator (2.243)

$$\begin{aligned} G(\mathbf{x},\tau;\mathbf{x}',\tau') &= \Theta(\tau-\tau')\frac{1}{\sqrt{2\pi\hbar^2(\tau-\tau')/M}^3} e^{-M(\mathbf{x}-\mathbf{x}')^2/2\hbar^2(\tau-\tau')} \\ &= G(\mathbf{x}-\mathbf{x}',\tau-\tau'). \end{aligned} \tag{2.393}$$

This Gaussian function coincides with the end-to-end distribution of a random walk of length proportional to $\hbar(\tau-\tau')$. Thus the quantum-mechanical propagator is a complex version of a particle performing a random walk. The random walk is caused by *quantum fluctuations*. This fluctuation picture of Schrödinger theory is exhibited best in the path integral formulation of quantum mechnics.[9] In the imaginary-time formulation of quantum field theory, we describe ensembles of particles. They correspond therefore to ensembles of random walks of fixed length. For this reason, nonrelativistic quantum field theories can be used efficiently to formulate theories of fluctuating polymers. In this context, they are called *disorder field theories*.[10] These will be discussed in Chapter 19.

Appendix 2A Permutation Group and Representations on n-Particle Wave Functions

A permutation of n particles is given by

$$P = \begin{pmatrix} 1 & 2 & \dots & n \\ p(1) & p(2) & \dots & p(n) \end{pmatrix}, \tag{2A.1}$$

where $p(i)$ are all possible one-to-one mappings of the integers $1,2,3,\dots,n$ onto themselves. In the notation (2A.1) the order of the columns is irrelevant, i.e., the same permutation can be written in any other form in which the columns are interchanged with each other, for example,

$$P = \begin{pmatrix} 2 & 1 & \dots & n \\ p(2) & p(1) & \dots & p(n) \end{pmatrix}. \tag{2A.2}$$

Given n particles at positions $\mathbf{x}_1,\mathbf{x}_2,\dots,\mathbf{x}_n$, the permutation P may be taken to change the position $\mathbf{x}_1$ to $\mathbf{x}_{p(1)}$, $\mathbf{x}_2$ to $\mathbf{x}_{p(2)}$, etc., i.e. we define P to act directly on the indices:

$$P\mathbf{x}_i \equiv \mathbf{x}_{p(i)}. \tag{2A.3}$$

Given an n-particle wave function $\psi(\mathbf{x}_1,\mathbf{x}_2,\dots,\mathbf{x}_n;t)$, it behaves under P as follows:

$$\begin{aligned} P\psi(\mathbf{x}_1,\mathbf{x}_2,\dots,\mathbf{x}_n;t) &= \psi(P\mathbf{x}_1,P\mathbf{x}_2,\dots,P\mathbf{x}_n;t) \\ &= \psi(\mathbf{x}_{p(1)},\mathbf{x}_{p(2)},\dots,\mathbf{x}_{p(n)};t). \end{aligned} \tag{2A.4}$$

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[9] See the textbook in Footnote 8.

[10] For details see the textbook quoted in Footnote 8 and H. Kleinert, *Gauge Fields in Condensed Matter*, World Scientific, 1989 (http://www.physik.fu-berlin.de/~kleinert/kleiner_re.html#b1).

There exists a different but equivalent definition of permutations, call them P', in which the variables $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ of the wave functions are taken from their places $1, 2, \ldots, n$ in the list of arguments of $\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n; t)$ and moved to the positions $p(1), p(2), \ldots, p(n)$ in this list, i.e.,

$$P'\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n; t) \equiv \psi(\ldots, \mathbf{x}_1, \ldots, \mathbf{x}_2, \ldots; t) \tag{2A.5}$$

where $\mathbf{x}_1$ is now at position $p(1)$, $\mathbf{x}_2$ at position $p(2)$, etc. The difference between the two definitions is seen in the following example:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; t) = \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1; t), \tag{2A.6}$$

to be compared with

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}' \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3; t) = \psi(\mathbf{x}_3, \mathbf{x}_1, \mathbf{x}_2; t). \tag{2A.7}$$

In the following we shall use only the first definition but all statements to be derived would hold as well if we were to use the second one throughout the remainder of this appendix.

For n elements there are $n!$ different permutations P. Given any two permutations

$$P = \begin{pmatrix} 1 & \ldots & n \\ p(1) & \ldots & p(n) \end{pmatrix}$$

and

$$Q = \begin{pmatrix} 1 & \ldots & n \\ q(1) & \ldots & q(n) \end{pmatrix},$$

a product is defined by rewriting Q as

$$Q = \begin{pmatrix} p(1) & \ldots & p(n) \\ q(p(1)) & \ldots & q(p(n)) \end{pmatrix}$$

and setting:

$$\begin{aligned} QP &\equiv \begin{pmatrix} p(1) & \ldots & p(n) \\ q(p(1)) & \ldots & q(p(n)) \end{pmatrix} \begin{pmatrix} 1 & \ldots & n \\ p(1) & \ldots & p(n) \end{pmatrix} \\ &\equiv \begin{pmatrix} 1 & \ldots & n \\ q(p(1)) & \ldots & q(p(n)) \end{pmatrix}. \end{aligned} \tag{2A.8}$$

Every element has an inverse since if we apply first P and multiply it by

$$P^{-1} \equiv \begin{pmatrix} p(1) & \ldots & p(n) \\ 1 & \ldots & n \end{pmatrix}, \tag{2A.9}$$

the operation $P^{-1}P$ returns all elements to their original places:

$$P^{-1}P=\begin{pmatrix} p(1) & \dots & p(n) \\ 1 & \dots & n \end{pmatrix}\begin{pmatrix} 1 & \dots & n \\ p(1) & \dots & p(n) \end{pmatrix}=\begin{pmatrix} 1 & \dots & n \\ 1 & \dots & n \end{pmatrix}\equiv I. \tag{2A.10}$$

The right-hand side is defined as the *identity permutation* I.

It can easily be checked that for three permutations PQR, the product is associative:

$$P(QR) = (PQ)R \tag{2A.11}$$

Thus the $n!$ permutations of n elements form a group, also called the *symmetric group* S_n.

If P is such that only two elements $p(i)$ are different from i it can be written as

$$T_{ij} = \left\{ \begin{matrix} 1 & 2 & \dots & i & \dots & j & \dots & n \\ 1 & 2 & \dots & p(i) & \dots & p(j) & \dots & n \end{matrix} \right\} \tag{2A.12}$$

and is called a *transposition*, also denoted in short by (i, j). Only the elements i and j are interchanged. Every permutation can be decomposed into a product of transpositions. There are many ways of doing this. However, each permutation decomposes either into an even or an odd number of transpositions. Therefore each permutation can be characterized by this property. It is also called the *parity* of the permutation. It is useful to introduce a function

$$\epsilon_P = \left\{ \begin{matrix} 1 \\ -1 \end{matrix} \right\} \text{for} \left\{ \begin{matrix} P=\text{even} \\ P=\text{odd} \end{matrix} \right\} \tag{2A.13}$$

which indicates the parity. This function satisfies the identity

$$\epsilon_{PQ} \equiv \epsilon_P \epsilon_Q, \tag{2A.14}$$

since, if P and Q are decomposed into transpositions,

$$P = \prod_{(ij)} T_{(ij)}, \qquad n \text{ factors} \tag{2A.15}$$

$$Q = \prod_{(i'j')} T_{(i'j')}, \qquad m \text{ factors,}$$

then the product

$$PQ = \prod_{(ij)} \prod_{(i'j')} T_{(ij)} T_{(i'j')} \tag{2A.16}$$

contains $n \times m$ transpositions. This number is even for n, m both even or odd, and odd if one of them is odd and the other even. Since the identity is trivially even, the inverse P^{-1} of a permutation has the same parity as P itself, i.e.,

$$\epsilon_{P^{-1}} = \epsilon_P. \tag{2A.17}$$

Let us find the irreducible representations of the permutation group on the Hilbert space of n-particle wave functions. The permutation on this space is defined by (2A.4). The irreducible representations can be classified with the help of the so-called *Young tableaux*. These are arrays of n boxes of the form

$$\begin{array}{l} \boxed{1}\boxed{2}\boxed{3}\boxed{4}\boxed{5}\boxed{6}\\ \boxed{7}\boxed{8}\boxed{9}\boxed{\cdot}\boxed{\cdot}\\ \boxed{\cdot}\boxed{\cdot}\boxed{\cdot}\\ \boxed{\cdot}\boxed{\cdot}\boxed{\cdot}\\ \boxed{\cdot}\boxed{\cdot}\\ \boxed{\cdot}\\ \boxed{\mathrm{n}}. \end{array} \tag{2A.18}$$

The boxes are filled successively with the numbers 1 to n. The numbers of boxes in the rows $m_1, m_2, m_3, \dots$ are ordered as

$$m_1 \geq m_2 \geq m_3 \geq \dots \qquad \sum_{k=1}^{n} m_k = n.$$

Each tableaux defines a symmetry type of the wave functions on which the group of permutations is represented irreducibly. The symmetry types are constructed as follows. Let p_i be all permutations, including the identity, of the numbers in the row i, and q_j the corresponding operations in the column j. Then define

$$\begin{aligned} P &= \textstyle\prod_i (\sum p_i), \\ Q &= \textstyle\prod_j (\sum \epsilon_{q_j} q_j), \end{aligned}$$

where the product is taken over all rows i or all columns j, respectively, and ϵ_q is the parity function (2A.13). Now apply the operation QP to the *indices* of the wave function $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$.

As an example, take the Hilbert space of three-particle wave functions. There are three different Yang tableaux corresponding to the following irreducible representations of S_3:

$$\boxed{1}\boxed{2}\boxed{3} \qquad P = \sum p \text{ (sum over all 6 elements of } S_3), \;\; Q = 1$$

$$\begin{array}{l}\boxed{1}\boxed{2}\\ \boxed{3}\end{array} \qquad P = 1 + (1,2), \quad Q = 1 - (1,3)$$

$$\begin{array}{l}\boxed{1}\\ \boxed{2}\\ \boxed{3}\end{array} \qquad P = 1, \;\; Q = \sum \epsilon_q q \text{ (sum over all 6 elements of } S_3)$$

The wave functions associated with these have the form

$$\boxed{1}\boxed{2}\boxed{3}\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \psi(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_1)$$

$$\begin{aligned} &+\psi(\mathbf{x}_3,\mathbf{x}_1,\mathbf{x}_2)+\psi(\mathbf{x}_1,\mathbf{x}_3,\mathbf{x}_2)\\ &+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_3)+\psi(\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_1), \end{aligned} \tag{2A.19}$$

$$\begin{aligned} \begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\end{array}\ \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) = {} & \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_3)\\ &-\psi(\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_1)-\psi(\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_1), \end{aligned} \tag{2A.20}$$

$$\begin{aligned} \begin{array}{l}\boxed{1}\\ \boxed{2}\\ \boxed{3}\end{array}\ \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) = {} & \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)+\psi(\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_1)\\ &+\psi(\mathbf{x}_3,\mathbf{x}_1,\mathbf{x}_2)-\psi(\mathbf{x}_1,\mathbf{x}_3,\mathbf{x}_2)\\ &-\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_3)-\psi(\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_1). \end{aligned} \tag{2A.21}$$

These wave functions are easily normalized by dividing them by the square root of the number of terms in each expression, i.e., $\sqrt{6}, 2, \sqrt{6}$, in the three cases. The horizontal array leads to the completely symmetrized, the vertical array to the completely antisymmetrized wave function. The second tableau results in a mixed symmetry.

Four-particle wave functions are classified with the following tableaux

$$\boxed{1}\boxed{2}\boxed{3}\boxed{4} + \begin{array}{lll}\boxed{1}&\boxed{2}&\boxed{3}\\ \boxed{4}&&\end{array}, + \begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\boxed{4}\end{array} + \begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\\ \boxed{4}&\end{array} + \begin{array}{l}\boxed{1}\\ \boxed{2}\\ \boxed{3}\\ \boxed{4}\end{array}. \tag{2A.22}$$

Take, for instance,

$$\begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\boxed{4}\end{array}$$

which amounts to the operator QP with

$$P=(1+(3,4))\,(1+(1,2))\,, \qquad Q=(1-(2,4))\,(1-(1,3))\,, \tag{2A.23}$$

so that

$$\begin{aligned} P\psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4) = {} & \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4)+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_3,\mathbf{x}_4)\\ &+\psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_4,\mathbf{x}_3)+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_4,\mathbf{x}_3),\\ QP\psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4) = {} & \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4)-\psi(\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_4)\\ &-\psi(\mathbf{x}_1,\mathbf{x}_4,\mathbf{x}_3,\mathbf{x}_2)+\psi(\mathbf{x}_3,\mathbf{x}_4,\mathbf{x}_1,\mathbf{x}_2)\\ &+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_3,\mathbf{x}_4)-\psi(\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_1,\mathbf{x}_4)\\ &-\psi(\mathbf{x}_4,\mathbf{x}_1,\mathbf{x}_3,\mathbf{x}_2)+\psi(\mathbf{x}_4,\mathbf{x}_3,\mathbf{x}_1,\mathbf{x}_2)\\ &+\psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_4,\mathbf{x}_3)-\psi(\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_4,\mathbf{x}_1)\\ &-\psi(\mathbf{x}_1,\mathbf{x}_4,\mathbf{x}_2,\mathbf{x}_3)+\psi(\mathbf{x}_3,\mathbf{x}_4,\mathbf{x}_2,\mathbf{x}_1)\\ &+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_4,\mathbf{x}_3)-\psi(\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4,\mathbf{x}_1)\\ &-\psi(\mathbf{x}_4,\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)+\psi(\mathbf{x}_4,\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_1). \end{aligned}$$

There exists an alternative but mathematically equivalent prescription of forming the wave functions of different symmetry types based on the permutations P' introduced in (2A.5) which, instead of performing the permutations on the indices exchanges the positions of the arguments in the wave functions $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_i,\ldots,\mathbf{x}_j,\ldots,\mathbf{x}_n)$. As an example, take the tableaux

$$\begin{array}{l}\boxed{1}\boxed{2}\\ \boxed{3}\end{array}$$

which gives with the alternative wave function

$$\begin{array}{l}\boxed{1}\boxed{2}\\ \boxed{3}\end{array}' \quad \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) = \psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)+\psi(\mathbf{x}_2,\mathbf{x}_1,\mathbf{x}_3) -\psi(\mathbf{x}_3,\mathbf{x}_2,\mathbf{x}_1)-\psi(\mathbf{x}_3,\mathbf{x}_1,\mathbf{x}_2)$$

rather than (2A.20).

The dimensionality with which the group elements of the permutation group are represented for these symmetry classes are given by the formula

$$d=\frac{n!}{\prod_{i,j}h_{ij}}, \tag{2A.24}$$

where h_{ij} is the number of boxes to the right of the position ij plus the number of boxes below the position ij in the tableaux, plus 1 for the box on the position ij itself.

As a useful check for the calculated dimensions we may use the *dimensionality theorem*, by which the squares of the dimensions d of all inequivalent, irreducible, unitary representations add up to the order of the group, here $n!$:

$$\sum d^2 = n!\ . \tag{2A.25}$$

This is a direct consequence of the *great orthogonality theorem* of such representations for any finite group.

For the permutation group at hand, one has the additional property that the defining representation contains each irreducible representation with a multiplicity equal to its dimension.

For three particles, the symmetric and antisymmetric representations

$$\boxed{}\boxed{}\boxed{}$$

and

$$\begin{array}{c}\boxed{}\\ \boxed{}\\ \boxed{}\end{array}$$

are $3!/3\times 2\times 1 = 1$-dimensional. The mixed representation

$$\begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}$$

is $3!/3 \times 1 \times 1 = 2$-dimensional. These dimensions fulfill the dimensionality formula (2A.25):

$$1^2 + 1^1 + 2^2 = 3! \, . \tag{2A.26}$$

Similarly one has for four particles the dimensionalities

$$\begin{array}{ll}
\begin{array}{l}\boxed{1}\boxed{2}\boxed{3}\boxed{4}\end{array} & d = \dfrac{4!}{4 \times 3 \times 2 \times 1} = 1, \\[2ex]
\begin{array}{l}\boxed{1}\boxed{2}\boxed{3} \\ \boxed{4}\end{array} & d = \dfrac{4!}{4 \times 2 \times 1 \times 1} = 3, \\[2ex]
\begin{array}{l}\boxed{1}\boxed{2} \\ \boxed{3}\boxed{4}\end{array} & d = \dfrac{4!}{3 \times 2 \times 2 \times 1} = 2, \\[2ex]
\begin{array}{l}\boxed{1}\boxed{2} \\ \boxed{3} \\ \boxed{4}\end{array} & d = \dfrac{4!}{4 \times 1 \times 2 \times 1} = 3, \\[2ex]
\begin{array}{l}\boxed{1} \\ \boxed{2} \\ \boxed{3} \\ \boxed{4}\end{array} & d = \dfrac{4!}{4 \times 3 \times 2 \times 1} = 1.
\end{array} \tag{2A.27}$$

Again we check that these dimensions fulfill the dimensionality formula (2A.25):

$$1^2 + 3^2 + 2^2 + 3^2 + 1^2 = 4! \, . \tag{2A.28}$$

Notes and References

For the second quantization in many-body physics and applications see
A.A. Abrikosov, L.P.Gorkov, and I.E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, Dover, 1963; A. Fetter and J.D. Walecka, *Quantum Theory of Many Particle Systems*, McGraw-Hill, New York, 1971.

The particles which obey neither bosonic nor fermionic statistics are explained in more detail and with many references in
H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* World Scientific, Singapore 2002. (http://www.physik.fu-berlin.de/~kleinert/kleiner_re.html#b7).

Good textbooks on statistical physics are
L.D. Landau and E.M. Lifshitz, *Statistical Physics*, Pergamon, New York, 1958;
R. Kubo, *Statistical Mechanics*, North-Holland, Amsterdam, 1971;
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For representations of finite groups and, in particular, the permutation group see
H. Boerner, *Darstellungen von Gruppen, mit Berücksichtigung der Bedürfnisse der*

modernen Physik, Springer, Berlin, 1055;
A.O. Barut and R. Raczka, *Theory of Group Representations and Applications*, World Scientific, Singapore, 1986;
M. Hamermesh, *Group Theory and its Application to Physical Problems*, Dover, New York, 1989;

3

Relativistic Free Fields

Having learned how many-particle Schrödinger theory can be reformulated as a quantum field theory, we shall now try to find possible field theories for the description of relativistic many-particle systems. This will first be done classically. The fields will be quantized in Chapter 5.

3.1 RELATIVISTIC PARTICLES

The nonrelativistic energy-momentum relation used in the Schrödinger theory

$$\varepsilon(\mathbf{p}) = \frac{\mathbf{p}^2}{2M} \tag{3.1}$$

is valid only for massive particles which move very much slower than the velocity of light[1]

$$c = 2.99792458 \times 10^{10}\text{cm/sec}. \tag{3.2}$$

If particles are accelerated to large velocities close to c this condition is no longer fulfilled. Instead of (3.1), the energy follows the relativistic law

$$\varepsilon(\mathbf{p}) = \sqrt{c^2\mathbf{p}^2 + c^4M^2}. \tag{3.3}$$

In particular, the light particles themselves, the photons, follow this law with the mass $M = 0$. It will be convenient to replace the energy by the new variable

$$p^0 \equiv \varepsilon(\mathbf{p})/c. \tag{3.4}$$

Then the relation (3.3) can be expressed as

$${p^0}^2 - \mathbf{p}^2 = M^2c^2. \tag{3.5}$$

Thus, energy and momentum of a particle of mass are always such that the *four-vector*

$$p^\mu = (p^0, p^i) \tag{3.6}$$

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[1] Note that since 1983 this has become a definition amounting to a redefinition of the meter as adopted by the Conférence Générale des Poids et Mesures. For a discussion see B.W. Petley, Nature *303*, 373 (1983).

is situated on the upper, $p^0 > 0$, hyperboloid in a four-dimensional energy-momentum space. This is called the *mass shell* of the particle of mass M. If the particles are massless, the hyperboloid degenerates into a cone, the so-called *light cone*.

Since a free particle remains free when seen from any rotated or uniformly moving coordinate frame, energy and momentum must transform in such a way as to remain always on the same mass shell. For a simple rotation of the frame this is obvious. The energy remains the same while the momentum **p** changes only its direction. For example, **p** may appear rotated around the z-axis by a transformation

$$p'^i = R_3(\varphi)^i{}_j p^j, \tag{3.7}$$

where $R_3(\varphi)$ is the matrix

$$R_3(\varphi) \equiv \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

The angle φ is defined in such a way that in the new rotated frame the momentum of the same particle appears rotated in the xy-plane in the anticlockwise direction, i.e., the coordinate axis have been rotated clockwise with respect to the original frame. We speak of a *passive* rotation of the system. The effect is the same as if the observer had remained in the same frame but rotated the experimental apparatus, and thereby the particle orbit, in the anticlockwise sense. The transformations defined in this way are called *active* transformations. There are two equivalent ways of formulating all invariance principles either in the active or in the passive way. In this text we shall use the passive way. The reader should be aware that different texts use different conventions and the formulas calculated in one cannot always be compared directly with those in the other but may require changes, which fortunately are quite straightforward.

For a general rotation by an angle φ with an axis pointing in the direction of the unit vector[2] $\hat{\boldsymbol{\varphi}}$, the transformation has the matrix form

$$p'^i = R_{\hat{\boldsymbol{\varphi}}}(\varphi)^i{}_j p^j, \tag{3.9}$$

which can also be written explicitly as

$$\mathbf{p}' = \cos\varphi\,\mathbf{p}_\perp + \sin\varphi\,(\hat{\boldsymbol{\varphi}} \times \mathbf{p}) + \mathbf{p}_{||}. \tag{3.10}$$

Here $\mathbf{p}_{||}, \mathbf{p}_\perp$ are the projections parallel and orthogonal to the rotation axis $\hat{\boldsymbol{\varphi}}$:

$$\mathbf{p}_{||} \equiv (\mathbf{p}\cdot\hat{\boldsymbol{\varphi}})\,\hat{\boldsymbol{\varphi}}, \quad \mathbf{p}_\perp \equiv \mathbf{p} - \mathbf{p}_{||}, \tag{3.11}$$

respectively. The set of all rotations form a group called the *rotation group*.

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[2] Hats on vectors in this section denote unit vectors, not Schrödinger operators.

Consider now another set of transformations in which the second frame moves with velocity v into the $-z$-direction of the first. Then in the new frame the z momentum of the particle will appear increased. The particle appears *boosted* in the z-direction with respect to the original observer. The momenta in x- and y-directions are unaffected. Since the total four-momentum still satisfies the mass shell condition (3.3), (3.5), the combination ${p^0}^2 - {p^3}^2$ has to remain invariant. This implies that there must be a hyperbolic transformation mixing p^0 and p^3 which may be parametrized by a hyperbolic angle ζ, called *rapidity*:

$$\begin{aligned} p'^0 &= \cosh\zeta\, p^0 + \sinh\zeta\, p^3, \\ p'^3 &= \sinh\zeta\, p^0 + \cosh\zeta\, p^3. \end{aligned} \tag{3.12}$$

This is called a pure Lorentz transformation. We may write this transformation in a 4×4 matrix form as

$$p'^\mu = \begin{pmatrix} \cosh\zeta & 0 & 0 & \sinh\zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh\zeta & 0 & 0 & \cosh\zeta \end{pmatrix}^{\mu}_{\ \ \nu} p^\nu \equiv B_3(\zeta)^\mu{}_\nu p^\nu. \tag{3.13}$$

The subscript 3 of B_3 indicates that the particle is boosted into the z-direction. A similar matrix can be written down for x and y-directions. In an arbitrary direction $\hat{\boldsymbol{\zeta}}$, the matrix elements are

$$B_{\hat{\zeta}}(\zeta) = \left(\begin{array}{c|c} \cosh\zeta & \hat{\zeta}^i \sinh\zeta \\ \hline \hat{\zeta}^i \sinh\zeta & \delta^{ij} + \hat{\zeta}^i\hat{\zeta}^j(\cosh\zeta - 1) \end{array} \right). \tag{3.14}$$

The spatial velocity of a particle is given by

$$\mathbf{v} \equiv \partial\varepsilon(\mathbf{p})/\partial\mathbf{p}. \tag{3.15}$$

In Schrödinger theory this is the velocity of a wave packet. In terms of $v \equiv |\mathbf{v}|$, one defines the *Einstein parameter*

$$\gamma \equiv \frac{1}{\sqrt{1 - v^2/c^2}} = \cosh\zeta. \tag{3.16}$$

In terms of these quantities, we can rewrite (3.14) as

$$B_{\hat{\mathbf{v}}}(v) = \left(\begin{array}{c|c} \gamma & \gamma v^i/c \\ \hline \gamma v^i/c & \delta^{ij} + (\gamma - 1)v^i v^j/v^2 \end{array} \right), \tag{3.17}$$

where $(\gamma - 1)v^i v^j/v^2$ is often conveniently rewritten as $\gamma^2 v^i v^j/c^2(\gamma - 1)$.

By combining rotations and boosts one obtains a 6-parameter manifold of matrices

$$\Lambda(\boldsymbol{\zeta}, \boldsymbol{\varphi}) = B_{\hat{\zeta}}(\zeta) R_{\hat{\varphi}}(\varphi). \tag{3.18}$$

These are called *proper Lorentz transformations*. For all these, the combination

$$p'^{0^2} - \mathbf{p}'^2 = p^{0^2} - \mathbf{p}^2 = M^2c^2 \tag{3.19}$$

is an invariant. These matrices form a group, the *proper Lorentz group*. We can easily see that the Lorentz group allows reaching *every* momentum p^μ on the mass shell by applying an appropriate group element to some *fixed* reference momentum p_R^μ. For example, if the particle has a mass M we may choose for p_R^μ the so-called *rest momentum*

$$p_R^\mu = (Mc, 0, 0, 0), \tag{3.20}$$

and apply the boost in the $\hat{\mathbf{p}}$-direction

$$\Lambda(\boldsymbol{\zeta}) = B_{\hat{\boldsymbol{\zeta}}}(\zeta), \tag{3.21}$$

with the rapidity given by

$$\cosh\zeta = \frac{p^0}{Mc}, \quad \sinh\zeta = \frac{|\mathbf{p}|}{Mc}. \tag{3.22}$$

With this, we can rewrite the general boost matrix (3.14) in the pure momentum form

$$B_{\hat{\mathbf{p}}}(|\mathbf{p}|) = \left(\begin{array}{c|c} p^0/M & |\mathbf{p}|p^i/M^2c^2 \\ \hline p^i|\mathbf{p}|/M^2c^2 & \delta^{ij} + \hat{p}^i\hat{p}^j\left(p^0/M - 1\right) \end{array}\right). \tag{3.23}$$

Instead of (3.21), we may choose the following more general boost in the $\hat{\mathbf{p}}$-direction $\Lambda(p) = B_{\hat{\mathbf{p}}}(|\mathbf{p}|)R_{\hat{\boldsymbol{\varphi}}}(\varphi)$, where $R_{\hat{\boldsymbol{\varphi}}}(\varphi)$ is an arbitrary rotation, since these leave the rest momentum p_R^μ invariant. In fact, the rotations form the largest subgroup of the group of all proper Lorentz transformations which leaves the rest momentum p_R^μ invariant. It is referred to as the *little group* or *Wigner group* of a massive particle. It has an important physical significance since it serves to specify the intrinsic rotational degrees of freedom of the particle. If the particle is at rest it carries no orbital angular momentum. If it happens that its quantum mechanical state remains completely invariant under the little group R, the particle must also have zero intrinsic angular momentum or zero *spin*. Besides this trivial representation, the little group being a rotation group can have representations of any angular momentum $s = \frac{1}{2}, 1, \frac{3}{2}, \ldots$. In these cases, the state at rest has $2s + 1$ components which are linearly recombined with each other upon rotations.

The situation is quite different in the case of massless particles. They move with the speed of light and p^μ cannot be brought by a Lorentz transformation from the light cone to a rest frame. There is, however, another standard reference momentum from which one can generate all other momenta on the light cone. It is given by

$$p_R^\mu = (1, 0, 0, 1)|\mathbf{p}|, \tag{3.24}$$

with an arbitrary size of the spatial momentum $|\mathbf{p}|$. It remains invariant under a different little group, which is again a three-parameter subgroup of the Lorentz group. The little groups will be discussed in detail in Section 3.16.1.

It is useful to write the invariant expression (3.19) as a square of a four-vector p^μ formed with the metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \tag{3.25}$$

namely

$$p^2 = g_{\mu\nu} p^\mu p^\nu. \tag{3.26}$$

In general, we define a scalar product between any two vectors as

$$pp' \equiv g_{\mu\nu} p^\mu p'^\nu = p^0 p'^0 - \mathbf{p}\mathbf{p}'. \tag{3.27}$$

Following Einsteins summation convention, repeated greek indices are summed from zero to 3 [recall (2.99)]. A space with this scalar product is called *Minkowski space*. It is useful to introduce the covariant components of any vector v^μ as

$$v_\mu \equiv g_{\mu\nu} v^\nu. \tag{3.28}$$

Then the scalar product can also be written as

$$pp' = p_\mu p'^\mu. \tag{3.29}$$

With this notation the mass shell condition (3.19) for a particle before and after a Lorentz transformation reads simply

$$p'^2 = p^2 = M^2c^2. \tag{3.30}$$

Note that, apart from the minus signs in the metric (3.25), the mass shell condition $p^2 = p^{0^2} - p^{1^2} - p^{2^2} - p^{3^2} = M^2c^2$, left invariant by the Lorentz group, is completely analogous to the spherical condition $p^{4^2} + p^{1^2} + p^{2^2} + p^{3^2} = M^2c^2$ which is left invariant by the rotation group in a four-dimensional euclidean space. Both groups are parametrized by six parameters which are associated with linear transformations in the six planes $12, 23, 31; 10, 20, 30$ or $12, 23, 31; 14, 24, 34$, respectively. In the case of the four-dimensional euclidean space these are all rotations which form the group of *special orthogonal matrices* called SO(4). The letter S indicates the property *special*. A group is called *special* if all its transformation matrices have a unit determinant. By analogy, the proper Lorentz group is denoted by SO(1,3). The numbers indicate the fact that in the Minkowski metric (3.25), one diagonal element is equal to +1 and three are equal to −1.

The fact that all group elements are "special" follows from a direct calculation of the determinant of the matrices in (3.9) [with (3.10)] and (3.14).

How do we have to describe the quantum mechanics of a free relativistic particle in Minkowski space? Energy and momentum p^0 and $\mathbf{p}$ must be related to the time and space derivatives of particle waves in the usual way

$$\begin{aligned} \hat{p}^0 &= i\hbar\frac{\partial}{\partial ct} \equiv i\hbar\frac{\partial}{\partial x^0}, \\ \hat{p}^i &= -i\hbar\frac{\partial}{\partial x^i}. \end{aligned} \tag{3.31}$$

In relativistic notation we have

$$\hat{p}_\mu = i\hbar\frac{\partial}{\partial x^\mu}. \tag{3.32}$$

Together with the coordinates, they satisfy the canonical commutation rules

$$\begin{aligned} [\hat{p}^\mu, \hat{p}^\nu] &= 0, \\ [x^\mu, x^\nu] &= 0, \\ [\hat{p}^\mu, x^\nu] &= i\hbar g^{\mu\nu}. \end{aligned} \tag{3.33}$$

We expect a free particle with momentum $\mathbf{p}$ be described by a field $\phi(x)$ of the plane-wave type

$$f_p(x) \propto e^{-i(p^0x^0-p^ix^i)/\hbar} = e^{-ipx/\hbar}. \tag{3.34}$$

In contrast to the nonrelativistic case where we have used the same letter $\psi(\mathbf{x}, t)$ for plane wave functions and field [see (2.213)], we choose here a different letter. The advantage of doing this will become apparent in Chapter 5 where the fields are quantized, but where we shall omit the hats on the field operators, for brevity. If the same letters denote field operators and plane waves, expansions of field operators into plane waves generalizing Eq. (2.216) would look confusing.

At this point we do not yet normalize the wave functions since we must first find a proper scalar product for calculating physical observables in these states. This scalar product will be given in (3.170).

We have stated previously that permissible energy momentum states of a free particle can be realized by considering *one and the same* particle in different coordinate frames connected by a transformation Λ. Suppose that we change the coordinates of the same spacetime point as follows:

$$x \to x' = \Lambda x. \tag{3.35}$$

Under this transformation the scalar product of any two vectors remains invariant:

$$x'y' = xy. \tag{3.36}$$

For rotations, this is obvious since $xy = x^0y^0 - \mathbf{x}\cdot\mathbf{y}$. For Lorentz transformations this is a direct consequence of the fact that the boost matrix (3.13) satisfies the relation

$$g_{\mu\mu'}B_3(\zeta)^\mu{}_\nu B_3(\zeta)^{\mu'}{}_\lambda = g_{\mu\lambda}, \tag{3.37}$$

or in matrix notation

$$B_3^T(\zeta)gB_3(\zeta) = g. \tag{3.38}$$

The same realtion holds obviously for the arbitrary boost matrix (3.14), and after a combination with all rotations for the general Lorentz transformation (3.18):

$$\Lambda^T g\Lambda = g, \tag{3.39}$$

or

$$g_{\mu\nu}\Lambda^\mu{}_\lambda\Lambda^\nu{}_\kappa = g_{\lambda\kappa}, \tag{3.40}$$

The invariance (3.36) of the scalar product is then verified in matrix notation as follows:

$$x'y' \equiv x'^T gy' = (\Lambda x)^T g(\Lambda y) = x^T\Lambda^T g\Lambda y = x^T y = xy. \tag{3.41}$$

This holds also for scalar products between momentum and coordinate vectors

$$p'x' = px. \tag{3.42}$$

If the metric were euclidean, this would be the definition of orthogonal matrices. In fact, in the notation (3.41) of scalar products in which the metric is suppressed, we may write

$$(\Lambda p)(\Lambda x) = p\Lambda^{-1}\Lambda x = px, \tag{3.43}$$

so that there is no difference between the manipulation of orthogonal and Lorentz matrices.

When changing spacetime coordinates from x to $x' = \Lambda x$, the plane wave function of a particle behaves like

$$f_p(x) = \text{const}\, e^{-ip\Lambda^{-1}x'/\hbar} = \text{const}\, e^{-i(\Lambda p)x'/\hbar} = f_{\Lambda p}(x') = f_{p'}(x'). \tag{3.44}$$

This shows that in the new coordinates the same particle appears with different momentum components

$$p' = \Lambda p. \tag{3.45}$$

Consider now an observable field $\phi(x)$ describing a particle which does not possess any intrinsic orientational degree of freedom, i.e., no spin. The field can be an arbitrary superposition of different plane wave functions $f_p(x)$. After a coordinate transformation it will still have the same value at the same spacetime point. Thus $\phi'(x')$ as seen in the new frame must be equal to $\phi(x)$ in the old frame, i.e.,

$$\phi'(x') = \phi(x). \tag{3.46}$$

A field with this property is called a *scalar field* or, for historical reasons, a *Klein-Gordon field*.[3]

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[3] O. Klein, Z. Phys. *37*, 895 (1926); V. Fock, ibid. *38*, 242; *39*, 226 (1926); W. Gordon, ibid. *40*, 117 (1926). Note that this name does injustice to E. Schrödinger. He actually invented the Klein-Gordon equation *first*, later his famous nonrelativistic wave equation, although his papers in Ann. Phys. *79*, 361, 489; *80*, 437; *81*, 109 (1926), suggest the opposite order, as pointed out by P.A.M. Dirac in *The Development of Quantum Theory*, Gordon and Breach, N.Y., 1971. See also Dirac's popular articles in Nature *189*, 335 (1961) and in Scientific American *208*, 45 (1963). When the spectrum of the hydrogen atom contradicted experiments, Schrödinger took the nonrelativistic limit of the Klein-Gordon equation and discovered the famous wave equation named after him.

3.2 DIFFERENTIAL OPERATORS FOR LORENTZ TRANSFORMATIONS

Equation (3.46) contains the same point of the physical system on both sides, labeled by different coordinates x and x'. For the derivation of consequences of symmetries (see Chapter 6) it is preferable to formulate the property (3.46) in the form of a transformation law at the same spacetime coordinates x (corresponding to different points of the physical system). Thus we shall express the transformation property (3.46) of a scalar field in the following form

$$\phi(x) \xrightarrow{\Lambda} \phi'_{\Lambda}(x) = \phi(\Lambda^{-1}x). \tag{3.47}$$

For clarity, we have marked the transformation producing $\phi'(x)$ by a subscript Λ. It is useful to realize that the inverse Lorentz transformation of the coordinates inside the field argument can also be achieved with the help of a differential operator. To find it we observe that the finite transformation matrices (3.9) and (3.17) can all be written in a convenient exponential form. We begin with the rotations. The four-dimensional form of the rotation (3.8) of the coordinate frame by an angle φ clockwise around the z-axis brings a point with coordinates x to new coordinates $x'^{\mu} = R_3(\varphi)^{\mu}{}_{\nu}x^{\nu}$ with the 4×4-matrix

$$R_3(\varphi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi & 0 \\ 0 & \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.48}$$

This can be written in the exponential form

$$R_3(\varphi) = \exp\left\{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\varphi\right\} \equiv e^{-iL_3\varphi}. \tag{3.49}$$

The matrix

$$L_3 = -i\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.50}$$

is called the *generator* of this rotation within the Lorentz group. Similarly we have for the x- and y-directions

$$L_1 = -i\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \tag{3.51}$$

$$L_2 = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{3.52}$$

For all three cases we may write the generators as

$$L_i \equiv -i \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \epsilon_{ijk} \end{array} \right), \tag{3.53}$$

where ϵ_{ijk} is the completely antisymmetric *Levi-Civita* tensor with $\epsilon_{123} = 1$. The pure rotation matrix (3.9) is given by the exponential

$$\Lambda = e^{-i\varphi \cdot \mathbf{L}}, \tag{3.54}$$

as can also be verified by expanding the exponential in a power series.

Let us now find the generators of the pure Lorentz transformations. First in the z-direction where we see from (3.13) that the boost matrix is

$$\begin{aligned} B_3(\zeta) &= \exp\left\{ \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \zeta \right\} \\ &= e^{-iM_3\zeta} \end{aligned} \tag{3.55}$$

with the generator

$$M_3 = i \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{3.56}$$

Similarly we have

$$M_1 = i \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{3.57}$$

$$M_2 = i \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.58}$$

The general Lorentz transformation matrix (3.14) is given by the exponential

$$\Lambda = e^{-i\zeta \cdot \mathbf{M}}, \tag{3.59}$$

as can be verified by expanding the exponential in a power series.

The full Lorentz group is therefore generated by the six matrices L_i, M_i, to be collectively denoted by $G_a (a = 1, \ldots, 6)$. Every element of the group can be written as

$$\Lambda = e^{-i(\boldsymbol{\varphi}\cdot\mathbf{L}+\boldsymbol{\zeta}\cdot\mathbf{M})} \equiv e^{-i\alpha_a G_a}. \tag{3.60}$$

If the exponential expanded in a power series, one reobtains for $\boldsymbol{\zeta} = \mathbf{0}$ or $\boldsymbol{\varphi} = \mathbf{0}$ the general transformation matrices (3.9) or (3.14), respectively.

There exists a Lorentz-covariant way of specifying the generators of the Lorentz group. We introduce the 4×4-matrices

$$(L^{\mu\nu})^{\lambda\kappa} = i(g^{\mu\lambda}g^{\nu\kappa} - g^{\mu\kappa}g^{\nu\lambda}), \tag{3.61}$$

labeled by the antisymmetric pair of indices $\mu\nu$, i.e.,

$$L^{\mu\nu} = -L^{\nu\mu}. \tag{3.62}$$

There are 6 independent matrices which coincide with the generators of rotations and boosts as follows:

$$L_i = \frac{1}{2}\epsilon_{ijk}L^{jk}, \tag{3.63}$$

$$M_i = L^{0i}. \tag{3.64}$$

With the generators (3.61), we can write every element (3.414) of the Lorentz group as follows

$$\Lambda = e^{-i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}}, \tag{3.65}$$

where the antisymmetric angular matrix $\omega_{\mu\nu} = -\omega_{\nu\mu}$ collects both, rotation angles and rapidities:

$$\omega_{ij} = \epsilon_{ijk}\varphi^k, \tag{3.66}$$

$$\omega_{0i} = \zeta^i. \tag{3.67}$$

Summarizing the notation we have set

$$\Lambda = e^{-i(\boldsymbol{\varphi}\cdot\mathbf{L}+\boldsymbol{\zeta}\cdot\mathbf{M})} = e^{-i(\frac{1}{2}\varphi^i\epsilon_{ijk}L^{jk}+\zeta^i L^{0i})} = e^{-i(\frac{1}{2}\omega_{ij}L^{ij}+\omega_{0i}L^{0i})} = e^{-i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}}. \tag{3.68}$$

Note that if the metric were euclidean

$$g = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \tag{3.69}$$

the situation would be well familiar from basic matrix theorems: Then Λ would comprise all real orthogonal matrices which could be written as an exponential of all real antisymmetric matrices. In our case only iL's are antisymmetric while iM are symmetric, a consequence of the minus signs in the Minkowski metric (3.25).

The reason for writing the group elements in this exponential form in terms of six generators is that by this the multiplication rules of infinitely many group elements can be completely reduced to the knowledge of the commutation rules among the six generators L_i, M_i. This is a consequence of the *Baker-Campbell-Hausdorff formula* written in the form[4]

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A-B,[A,B]]+\dots}. \tag{3.70}$$

According to this formula we have with the general notation $G_a = (L_i, M_i)$ for the six generators in Eqs. (3.53) and (3.56)–(3.58),

$$\begin{aligned}\Lambda_1\Lambda_2 &= e^{-i\alpha_a^1 G_a} e^{-i\alpha_b^2 G_b} \\ &= \exp\Big\{-i\alpha_a^1 G_a - i\alpha_b^2 G_b + \frac{1}{2}[-i\alpha_a^1 G_a, -i\alpha_b^2 G_b] \\ &\quad + \frac{1}{12}[-i(\alpha_c^1 - \alpha_c^2)G_c, [-i\alpha_a^1 G_a, -i\alpha_b^2 G_b]] + \dots\Big\}. \end{aligned} \tag{3.71}$$

The exponent involves only commutators among G_a's. For the Lorentz group these can be calculated from the explicit 4×4 -matrices (3.50)–(3.52) and (3.56)–(3.58). The result is

$$[L_i, L_j] = i\epsilon_{ijk} L_k, \tag{3.72}$$

$$[L_i, M_j] = i\epsilon_{ijk} M_k, \tag{3.73}$$

$$[M_i, M_j] = -i\epsilon_{ijk} L_k. \tag{3.74}$$

This algebra of generators is called the *Lie algebra* of the group. The number of linearly independent matrices G_a (here 6) is called the *rank* r of the Lie algebra. In the general notation with the generators G_a, the algebra reads

$$[G_a, G_b] = i f_{abc} G_c. \tag{3.75}$$

The commutator of two generators is a linear combination of generators. The coefficients f_{abc} are called *structure constants*. They are completely antisymmetric in a, b, c, and satisfy the relation

$$f_{abd} f_{dcf} + f_{bcd} f_{daf} + f_{cad} f_{dbf} = 0, \tag{3.76}$$

which guarantees that the generators obey the *Jacobi identity*

$$[[G_a, G_b], G_c] + [[G_b, G_c], G_a] + [[G_c, G_a], G_b] = 0, \tag{3.77}$$

which is the law of associativity for Lie Algebras. The relation (3.76) can easily be verified for the structure constants (3.72)–(3.74) using the identity for the ϵ-tensor

$$\epsilon_{ijl}\epsilon_{lkm} + \epsilon_{jkl}\epsilon_{lim} + \epsilon_{kil}\epsilon_{ljm} = 0. \tag{3.78}$$

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[4] For a derivation see Appendix 3A.

The Jacobi identity implies that the r matrices with $r \times r$ elements

$$(F_c)_{ab} \equiv -if_{cab} \tag{3.79}$$

satisfy the commutation rules (3.75). They form the so-called *adjoint representation* of the Lie algebra. The matrix (3.53) for L_i is precisely of this type.

In terms of the matrices F_a of the adjoint representation, the commutation rules can also be written as

$$[G_a, G_b] = -(F_c)_{ab} G_c. \tag{3.80}$$

Continuing the expansion in terms of commutators in the exponent of (3.71), the commutators can be executed successively and one remains at the end with an expression

$$\Lambda_{12} = e^{-i\alpha_a^{12}(\alpha^1,\alpha^2)G_a}, \tag{3.81}$$

with the parameters of the product α_a^{12} being completely determined from α_a^1, α_a^2 for any given structure constants f_{abc}.

In the tensor notation $L^{\mu\nu}$ for L_i, M_i of Eqs. (3.63), (3.64), and with multiplication performed covariantly, so that products $L^{\mu\nu}L^{\lambda\kappa}$ have the matrix elements $(L^{\mu\nu})_{\sigma\tau}(L^{\lambda\kappa})^{\tau}{}_{\delta}$, the commutators read

$$[L^{\mu\nu}, L^{\lambda\kappa}] = -i(g^{\mu\lambda}L^{\nu\kappa} - g^{\mu\kappa}L^{\nu\lambda} + g^{\nu\kappa}L^{\mu\lambda} - g^{\nu\lambda}L^{\mu\kappa}). \tag{3.82}$$

Due to the antisymmetry in $\mu \leftrightarrow \nu$ and $\lambda \leftrightarrow \kappa$ it is sufficient to specify only the simpler commutators

$$[L^{\mu\nu}, L^{\mu\lambda}] = -ig^{\mu\mu}L^{\nu\lambda}, \quad \text{no sum over } \mu, \tag{3.83}$$

thereby omitting vanishing components in (3.82) in which none of the indices $\mu\nu$ is equal to one of the indices $\lambda\kappa$.

After these preparations we are ready to derive a differential operator which achieves the transformation of the spacetime argument in (3.47). First we consider infinitesimal Lorentz matrices

$$\Lambda \equiv 1 - i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}. \tag{3.84}$$

The transformation

$$x \xrightarrow{\Lambda} x' = \Lambda x \tag{3.85}$$

can be written as an infinitesimal symmetry transformation

$$\delta_s x = x' - x = -i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}x. \tag{3.86}$$

Inserting the generators (3.61), this becomes more explicitly

$$\delta_s x^\mu = \omega^\mu{}_\nu x^\nu. \tag{3.87}$$

With this, the argument on the right-hand side of the field transformation law (3.47) reads $x^\mu - \omega^\mu{}_\nu x^\nu$, so that the infinitesimal transformation takes the form

$$\phi(x) \xrightarrow{\Lambda} \phi(x) + \delta_{\rm s}\phi(x), \quad \text{with} \quad \delta_{\rm s}\phi(x) = -\omega^\mu{}_\nu x^\nu \partial_\mu \phi(x). \tag{3.88}$$

Alternatively we can write

$$\delta_{\rm s}\phi(x) = -i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}\phi(x), \tag{3.89}$$

where $\hat{L}^{\mu\nu}$ are the differential operators

$$\hat{L}^{\mu\nu} \equiv i(x^\mu\partial^\nu - x^\nu\partial^\mu). \tag{3.90}$$

In terms of the quantum mechanical canonical momentum operators (3.32), this becomes

$$\hat{L}^{\mu\nu} \equiv \frac{1}{\hbar}(x^\mu\hat{p}^\nu - x^\nu\hat{p}^\mu). \tag{3.91}$$

The object in parentheses is the tensor version of the four-dimensional operator of angular momentum.

The operators (3.91) satisfy the same commutation relations (3.82), (3.83) as the 4 × 4 -generators $L^{\mu\nu}$ of the Lorentz group. They form a representation of the Lie algebra (3.82), (3.83) in terms of differential operators generating the Lorentz transformations on the spacetime argument of any field.

In working out the commutation rules among the differential operators $\hat{L}^{\mu\nu}$ one conveniently uses the commutation rules between $\hat{L}^{\mu\nu}$ and x^λ as well as $\hat{p}^\lambda$:

$$\begin{aligned} [\hat{L}^{\mu\nu}, x^\lambda] &= -i(g^{\mu\lambda}x^\nu - g^{\nu\lambda}x^\mu) = -(L^{\mu\nu})^\lambda{}_\kappa x^\kappa, && (3.92)\\ [\hat{L}^{\mu\nu}, \hat{p}^\lambda] &= -i(g^{\mu\lambda}\hat{p}^\nu - g^{\nu\lambda}\hat{p}^\mu) = -(L^{\mu\nu})^\lambda{}_\kappa \hat{p}^\kappa. && (3.93) \end{aligned}$$

These commutation rules identify x^λ and $\hat{p}^\lambda$ as vector operators [recall the definition in (2.111)]. In general, an operator $t^{\lambda_1,\cdots,\lambda_n}$ is said to be a tensor operator of rank n if it is transformed by $L^{\mu\nu}$ like x^μ or $\hat{p}^\mu$ in each tensor index:

$$\begin{aligned} [\hat{L}^{\mu\nu}, \hat{t}^{\lambda_1,\ldots,\lambda_n}] &= -i[(g^{\mu\lambda_1}\hat{t}^{\nu,\ldots,\lambda_n} - g^{\nu\lambda_1}\hat{t}^{\mu,\ldots,\lambda_n}) + \ldots + (g^{\mu\lambda_n}\hat{t}^{\lambda_1,\ldots,\nu} - g^{\nu\lambda_n}\hat{t}^{\lambda_1,\ldots,\mu})] \\ &= -(L^{\mu\nu})^{\lambda_1}{}_\kappa \hat{t}^{\kappa\lambda_2,\ldots,\lambda_n} - (L^{\mu\nu})^{\lambda_2}{}_\kappa \hat{t}^{\lambda_1\kappa,\ldots,\lambda_n} - (L^{\mu\nu})^{\lambda_n}{}_\kappa \hat{t}^{\lambda_1\lambda_2,\ldots,\kappa}. \end{aligned} \tag{3.94}$$

The simplest examples for such tensor operators are $\hat{t}^{\lambda_1,\ldots,\lambda_n} = x^{\lambda_1}\cdots x^{\lambda_n}$ or $\hat{t}^{\lambda_1,\ldots,\lambda_n} = \hat{p}^{\lambda_1}\cdots\hat{p}^{\lambda_n}$.

The commutators (3.82) between the generators imply that these, themselves, are tensor operators of rank 2.

It is worth observing that the differential operators $\hat{L}^{\mu\nu}$ can also be expressed in terms of the 4 × 4 matrix generators (3.61) as

$$\hat{L}^{\mu\nu} = \frac{i}{\hbar}(L^{\mu\nu})_{\lambda\kappa}x^\lambda\hat{p}^\kappa = \frac{i}{\hbar}x^T L^{\mu\nu}\hat{p} = -i\hat{p}^T L^{\mu\nu}x. \tag{3.95}$$

In this form, the operators $\hat{L}^{\mu\nu}$ follow the same algebraic construction rules as the operators $\hat{a}^\dagger M_i \hat{a}$ in Section 2.5. There we showed that sandwich constructions between creation and annihilation operators $\hat{a}^\dagger L^{\mu\nu}\hat{a}$ carry the commutation rules between the matrices $L^{\mu\nu}$ into a larger Hilbert space without changing the commutation rules. Since $-i\hat{p}_\mu$ and x^μ commute in the same way as $\hat{a}^\dagger$ and $\hat{a}$, the same argument applies to the sandwich construction (3.95), where the matrix generators $L^{\mu\nu}$ of Eq. (3.61) between $-i\hat{p}^\mu$ and x^ν produces an infinite-dimensional representation in terms of differential operators acting on the Hilbert space of square-integrable functions.

The commutation relations between the group generators (3.91) and vector and tensor operators can be used to calculate the effect of finite group transformations upon these operators. They can also be used to express the transformation property (3.46) in another way. A finite Lorentz transformation of a scalar field is obtained by exponentiating the generators just as in the 4 × 4 -representation (3.65) and (3.68). Thus we define the differential operator representation of finite group elements (3.65) as

$$\hat{D}(\Lambda) \equiv e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}. \tag{3.96}$$

Since the generators $\hat{L}^{\mu\nu}$ commute in the same way among each other as the 4 × 4 -matrix generators (3.61), the operators $\hat{D}(\Lambda)$ obey the same group multiplication rules as 4 × 4 -matrices Λ. This follows directly from the expansion (3.71) of the product in terms of commutators.

Let us apply such a finite transformation to the vector x^μ and form

$$\hat{D}(\Lambda)x^\lambda\hat{D}^{-1}(\Lambda). \tag{3.97}$$

We do this separately for rotations and Lorentz tranformations, first for rotations.

An arbitrary three-vector (x^1, x^2, x^3) is rotated around the 3-axis by the operator $\hat{D}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}$ with $\hat{L}_3 = -i(x^1\partial_2 - x^2\partial_1)$ by the operation

$$\hat{D}(R_3(\varphi))x^i\hat{D}^{-1}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}x^i e^{i\varphi\hat{L}_3}. \tag{3.98}$$

The right-hand side is evaluated with the help of *Lie's expansion formula*

$$e^{-i\hat{A}}\,\hat{B}\,e^{iA} = 1 - i[\hat{A},\hat{B}] + \frac{i^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \dots\ . \tag{3.99}$$

Since $\hat{L}_3$ commutes with x^3, this component is unchanged by the operation (3.107):

$$\hat{D}(R_3(\varphi))x^3\hat{D}^{-1}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}x^3 e^{i\varphi\hat{L}_3} = x^3. \tag{3.100}$$

For x^1 and x^2, the Lie expansion of (3.97) contains the commutators

$$-i[L_3, x^1] = x^2, \qquad -i[L_3, x^2] = -x^1. \tag{3.101}$$

Thus, the first-order expansion term transforms the two-dimensional vector (x^1, x^2) into $(x^2, -x^1)$. The second-order terms are obtained by commuting the operator

$-i\hat{L}_3$ with these components, yielding $-(x^1,x^2)$. To third-order, this is again transformed into $-(x^2,-x^1)$, and so on. Obviously, all even orders reproduce the initial two-dimensional vector (x^1,x^2) with an alternating sign, while all odd powers are proportional to $(x^2,-x^1)$:

$$\begin{aligned} e^{-i\varphi\hat{L}_3}(x^1,x^2)e^{i\varphi\hat{L}_3} &= \left(1-\frac{1}{2!}\varphi^2+\frac{1}{4!}\varphi^4+\dots\right)(x^1,x^2) \\ &+ \left(\varphi-\frac{1}{3!}\varphi^3+\frac{1}{5!}\varphi^5+\dots\right)(x^2,-x^1). \end{aligned} \tag{3.102}$$

The even and odd powers can be summed up, and we obtain

$$e^{-i\varphi\hat{L}_3}(x^1,x^2)e^{i\varphi\hat{L}_3} = \cos\varphi\;(x^1,x^2)+\sin\varphi\;(x^2,-x^1). \tag{3.103}$$

Together with (3.100), the right-hand side corresponds precisely to the *inverse* rotation (3.8). Thus

$$\hat{D}(R_3(\varphi))x^i\hat{D}^{-1}(R_3(\varphi)) = e^{-i\varphi\hat{L}_3}x^ie^{i\varphi\hat{L}_3} = x^jR_3(\varphi)_j{}^i = R_3^{-1}(\varphi)^i{}_jx^j. \tag{3.104}$$

By performing successively rotations around the three axes we can generate in this way any rotation.

$$\hat{D}(R_{\boldsymbol{\varphi}}(\varphi))x^i\hat{D}^{-1}(R_{\boldsymbol{\varphi}}(\varphi)) = e^{-i\boldsymbol{\varphi}\cdot\hat{\mathbf{L}}}x^ie^{i\boldsymbol{\varphi}\cdot\hat{\mathbf{L}}} = x^jR_{\boldsymbol{\varphi}}(\varphi)_j{}^i = R_{\boldsymbol{\varphi}}^{-1}(\varphi)^i{}_jx^j, \tag{3.105}$$

this being the finite rotation form of the commutation relation for the vector operator x^i:

$$[\hat{L}_i,x_k] = x_j(L_i)_{jk}, \tag{3.106}$$

which holds for any vector operator $\hat{v}^i$ replacing x^i [recall again the definition in (2.111)].

The time component x^0 is obviously unchanged by a rotation since $\hat{L}_3$ commutes with x^0.

A similar calculation may be done for pure Lorentz transformations. Here we first consider a boost in the 3-direction $B_3(\zeta) = e^{-i\zeta\hat{M}_3}$ generated by $\hat{M}_3 = \hat{L}^{03} = -i(x^0\partial_3+x^3\partial_0)$ [recall (3.68), (3.64), and (3.90)]. Note the positive relative sign of the two terms in the generator $\hat{L}^{03}$ caused by the fact that $\partial_i = -\partial^i$ in contrast to $\partial_0 = \partial^0$. Thus we form

$$\hat{D}(B_3(\zeta))x^i\hat{D}^{-1}(B_3(\zeta)) = e^{-i\zeta\hat{M}_3}x^ie^{i\zeta\hat{M}_3}. \tag{3.107}$$

The Lie expansion of the right-hand side involves the commutators

$$-i[M_3,x^0] = -x^3, \quad -i[M_3,x^3] = -x^0, \quad -i[M_3,x^1] = 0, \quad -i[M_3,x^2] = 0. \tag{3.108}$$

Thus the two-vector (x^1,x^2) is unchanged, while the two-vector (x^0,x^3) is transformed into $-(x^3,x^0)$. In the second expansion term, the latter becomes (x^0,x^3), and so on, yielding

$$\begin{aligned} e^{-i\zeta\hat{M}_3}(x^0,x^3)e^{i\zeta\hat{M}_3} &= \left(1+\frac{1}{2!}\zeta^2+\frac{1}{4!}\zeta^4+\dots\right)(x^0,x^3) \\ &- \left(\zeta+\frac{1}{3!}\zeta^3+\frac{1}{5!}\zeta^5+\dots\right)(x^3,x^0), \end{aligned} \tag{3.109}$$

which can be summed up

$$e^{-i\zeta\hat{M}_3}(x^0,x^3)e^{i\zeta\hat{M}_3} = \cosh\zeta\,(x^0,x^3) - \sinh\zeta\,(x^3,x^0). \tag{3.110}$$

Together with the invariance of (x^1,x^2), this corresponds precisely to the inverse of the boost transformation (3.13). Thus:

$$\hat{D}(B_3(\zeta))x^\mu\hat{D}^{-1}(B_3(\zeta)) = e^{-i\zeta\hat{M}_3}x^\mu e^{i\zeta\hat{M}_3} = B_3^{-1}(\zeta)^\mu{}_\nu x^\nu. \tag{3.111}$$

By performing successively rotations and boosts in all directions we find for the entire Lorentz group

$$\hat{D}(\Lambda)x^\lambda\hat{D}^{-1}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}x^\lambda e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} = (\Lambda^{-1})^\lambda{}_{\lambda'}x^{\lambda'} = (e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}})^\lambda{}_{\lambda'}x^{\lambda'}, \tag{3.112}$$

where $\omega_{\mu\nu}$ are the parameters (3.66) and (3.67). In the last term on the right-hand side we have expressed the 4×4 -matrix Λ as an exponential of its generators as well, to emphasize the one-to-one correspondence between the generators $L^{\mu\nu}$ and their differential-operator representation $\hat{L}^{\mu\nu}$.

At first it may seem surprising that the group transformations appearing as a left-hand factor of the two sides of these equations are *inverse* to each other. However, we may easily convince ourselves this is necessary to guarantee the correct group multiplication law. Indeed, if we perform two transformations after each other they appear in opposite order on the right- and left-hand sides:

$$\begin{aligned}&\hat{D}(\Lambda_2\Lambda_1)x^\lambda\hat{D}^{-1}(\Lambda_2\Lambda_1) = \hat{D}(\Lambda_2)\hat{D}(\Lambda_1)x^\lambda\hat{D}^{-1}(\Lambda_1)\hat{D}^{-1}(\Lambda_2)\\ &\quad= (\Lambda_1^{-1})^\lambda{}_{\lambda'}\hat{D}(\Lambda_2)x^{\lambda'}\hat{D}^{-1}(\Lambda_2) = (\Lambda_1^{-1})^\lambda{}_{\lambda'}(\Lambda_2^{-1})^{\lambda'}{}_{\lambda''}x^{\lambda''} = [(\Lambda_2\Lambda_1)^{-1}]^\lambda{}_{\lambda'}x^{\lambda'}.\end{aligned} \tag{3.113}$$

If the right-hand side of (3.112) would contain Λ instead of Λ^{-1}, the order of the factors in $\Lambda_2\Lambda_1$ on the right-hand side of (3.113) would be opposite to the order in $\hat{D}(\Lambda_2\Lambda_1)$ on the left-hand side.

A straightforward extension of the operation (3.112) yields the transformation law for a tensor $\hat{t}^{\lambda_1,\dots,\lambda_n} = x^{\lambda_1}\cdots x^{\lambda_n}$:

$$\begin{aligned}\hat{D}(\Lambda)\hat{t}^{\lambda_1,\dots,\lambda_n}\hat{D}^{-1}(\Lambda) &= e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\hat{t}^{\lambda_1,\dots,\lambda_n}e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\\ &= (\Lambda^{-1})^{\lambda_1}{}_{\lambda_1'}\cdots(\Lambda^{-1})^{\lambda_n}{}_{\lambda_n'}\hat{t}^{\lambda_1',\dots,\lambda_n'}\\ &= (e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}})^{\lambda_1}{}_{\lambda_1'}\cdots(e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}})^{\lambda_n}{}_{\lambda_n'}\hat{t}^{\lambda_1',\dots,\lambda_n'}.\end{aligned} \tag{3.114}$$

This follows directly by inserting in the product $x^{\lambda_1}\cdots x^{\lambda_n}$, an auxiliary unit factor $1 = \hat{D}(\Lambda)\hat{D}^{-1}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}$ between neighboring factors x^{λ_i} and performing the operation (3.114) on each of them. The last term in (3.114) can also be written as

$$\left[e^{i\frac{1}{2}\omega_{\mu\nu}(L^{\mu\nu}\times 1\times 1\cdots\times 1\ +\ \dots\ +\ 1\times L^{\mu\nu}\times 1\cdots\times 1)}\right]^{\lambda_1\dots\lambda_n}{}_{\lambda_1'\dots\lambda_n'}\ t^{\lambda_1'\dots\lambda_n'}.$$

Since the commutation relations (3.94) determine the result completely, the transformation formula (3.114) is true for any tensor operator $\hat{t}^{\lambda_1,\dots,\lambda_n}$ not only those composed from a product of vectors x^{λ_i}.

For a field $\phi(x)$ which can be expanded into a power series, the transformation law (3.114) generalizes immediately to

$$\hat{D}(\Lambda)\phi(x)\hat{D}^{-1}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\phi(x)e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} = \phi(\Lambda^{-1}x) = \phi(e^{i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}}x). \quad (3.115)$$

The finite transformation law (3.47) of a scalar field can therefore be expressed with the help of the differential operator $\hat{D}(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}$ as

$$\phi(x) \xrightarrow{\Lambda} \phi'_\Lambda(x) = \phi(\Lambda^{-1}x) = \hat{D}(\Lambda)\phi(x)\hat{D}^{-1}(\Lambda) \equiv e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\phi(x)e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}. \quad (3.116)$$

The last factor on the right-hand side can, of course, be omitted if there are no x-dependent functions behind it.

If a particle has spin degrees of freedom its field transforms differently from (3.116). Then the wave function has several components to account for the spin orientations. The transformation law must be such that the spin orientation in space remains the same at the same space point. This implies that the field components which specify the orientation with respect to the different coordinate axes will have to be transformed by certain matrices. How this is done for relativistic fields has first been understood for electromagnetic and gravitational fields which exhibit vector and tensor transformation properties, respectively. These will be recalled below, before generalizing them to the case of arbitrary spin.

3.3 SPACE INVERSION AND TIME REVERSAL

In addition to the continuous Lorentz transformations, there are also two important discrete transformations which leave scalar products $p_\mu x^\mu$ invariant. First there is the *space inversion*, also called *space reflection*, or *parity transformation*

$$P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \quad (3.117)$$

which reverses the direction of the spatial vectors, $\mathbf{x} \to -\mathbf{x}$. Note that a space inversion differs from a mirror reflection by a rotation. The space inversion maps the generators L_i, M_i of the Lorentz group into partiy transformed generators

$$L_i \xrightarrow{P} L_i^P \equiv PL_iP^{-1} = L_i, \qquad M_i \xrightarrow{P} M_i^P \equiv PM_iP^{-1} = -M_i. \quad (3.118)$$

This behavior is obvious in the tensor form of the generators $(L_i, M_i) = (\frac{1}{2}\epsilon_{ijk}L^{ik}, L^{0i})$: each spacelike index gives rise to a factor -1. The transformation preserves the commutation rules (3.73)–(3.74):

$$[L_i^P, L_j^P] = i\epsilon_{ijk}L_k^P, \quad (3.119)$$

$$[L_i^P, M_j^P] = i\epsilon_{ijk}M_k^P, \quad (3.120)$$

$$[M_i^P, M_j^P] = -i\epsilon_{ijk}L_k^P. \quad (3.121)$$

In general, a mapping of the generators into linear combinations of generators which have the same commutation rules is called an *automorphismus* of the Lie algebra.

Second there is the *time inversion* or *time reversal* transformation

$$T=\begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \tag{3.122}$$

which changes the sign of x^0. When applied to the generators of the defining representation (L_i, M_i), the time reversal transformation produces the same automorphism of the Lie algebra as the parity transformation (3.118). This, however, is a special feature of the reality of the Lorentz transformations Λ. This makes the 4×4-matrices of the generators (3.50)–(3.52) and (3.56)–(3.58) accidentally purely imaginary.

Physically, a process is invariant under time reversal if we are unable to judge whether a movie of the process runs forward or backward. Running it backward amounts to changing momentum and angular momentum L_i. Since momentum is generated by boost transformations, time reversal must change the direction of M_i. For hermitian matrices it is only necessary to change the eigenvalues, such that we can also require L_i going to $-L_i^*$. In fact, there is a natural automorpism of the Lie algebra (3.73)–(3.74) in which we simply take the complex conjugate of the commutation rules, bringing them to

$$\begin{aligned} [-L_i^*, -L_j^*] &= i\epsilon_{ijk}(-L_k^*), && (3.123)\\ [-L_i^*, -M_j^*] &= i\epsilon_{ijk}(-M_k^*), && (3.124)\\ [-M_i^*, -M_j^*] &= -i\epsilon_{ijk}(-L_k^*). && (3.125) \end{aligned}$$

As we shall see in detail below when discussing the time reversal properties of the various fields, this automorphism has precisely the desired observational consequences which we would like to associate with a time reversal transformation. Explicitly, time reversal transforms the generators as follows:

$$L_i \xrightarrow{T} L_i^T \equiv TL_iT^{-1} = -L_i^*, \qquad M_i \xrightarrow{T} M_i^T \equiv TM_iT^{-1} = -M_i^*. \tag{3.126}$$

If the operations P and T are incorporated into the special Lorentz group SO(1,3) one speaks of the *full Lorentz group*.

Note that the determinant of (3.117) and (3.122) is negative so that the full Lorentz group no longer deserves the letter S in its name. It is called $O(1,3)$.

3.4 RELATIVISTIC FREE SCALAR FIELDS

The question now arises as to how the nonrelativistic free-field action

$$\mathcal{A} = \int dt d^3x\, \psi^*(\mathbf{x},t) \left[i\hbar\partial_t + \frac{\hbar^2}{2M}{\partial_{\mathbf{x}}}^2 \right] \psi(\mathbf{x},t) \tag{3.127}$$

introduced in (2.203) has to be modified in order to permit a quantum mechanical description of arbitrary relativistic n-particle states. According to the definition in (2.161), this is a local action. A field theory based on a local action will be called *local field theory*. All field theories which explain successfully the properties of elementary particle have so far turned out to be local. The locality property seems to be extremely fundamental. All fundamental forces which historically have been found as bilocal forces (this used to be called *action at a distance forces*) have eventually been found to be the result of a local action involving an extra field mediating the interaction. In the case of electromagnetism, the Coulomb interaction which initially is described by a bilocal term in the action (see Section 2.8) can be reduced to a local interaction involving an extra potential field, which turns out to be a component of a vector potential describing the particles of light, the *photons* (see Chapter 10). The same thing holds for gravitational forces and the particles called *gravitons*. In nuclear physics, the locality principle has led Yukawa to the discovery of the fundamental particle called π-*meson* [see Section 22.3, in particular Eqs. (2.159) and (2.137) for $V_2(\mathbf{x}-\mathbf{x}') \propto 1/|\mathbf{x}-\mathbf{x}'|$].

In order to accommodate the kinematic features discussed in the last section we shall require the action to be invariant under Lorentz transformations (3.35), (3.46). Hence, space and time derivatives have to appear on equal footing, i.e., both must appear linearly or quadratically and with no higher power than that if we want to maintain the usual principle of classical mechanics in which all differential equations are of second order in time. Depending on the possible internal spin degrees of freedom there are different ways of making the action relativistic. These will now be discussed separately.

Consider first a field associated with a relativistic point particle which carries no spin degree of freedom, thus avoiding a nontrivial behavior under space rotations. Such a field is called a *scalar field* and will be denoted by $\phi(x)$. As in the nonrelativistic case, the action of this field must contain the square of the spatial derivatives ∂_i to guarantee rotational invariance. Since there must be Lorentz symmetry between spatial and time derivatives, we are led to a classical local action

$$\begin{aligned} \mathcal{A} = \int dx^0 L &= \int dx^0 d^3x\, \phi^*(\mathbf{x},t) \left[-c_1\hbar^2(\partial_0^2 - \partial_{\mathbf{x}}^2) - c_2\right] \phi(\mathbf{x},t) \\ &= \int d^4x\, \phi^*(x) \left[-c_1\hbar^2\partial^\mu\partial_\mu - c_2\right] \phi(x), \end{aligned} \tag{3.128}$$

where $c_1\hbar^2, c_2$ are two arbitrary real constants.

It is easy to see that this action is indeed Lorentz invariant: Under the transformation (3.35), the four-volume element does not change

$$dx^0 d^3x \equiv d^4x \to d^4x' = d^4x. \tag{3.129}$$

This follows directly from Eq. (3.39) which imples that $\det \Lambda = \pm 1$ If we therefore take the action in the new frame

$$\mathcal{A} = \int d^4x'\, \phi^{*\prime}(x') \left[-c_1\hbar^2\partial'^\mu\partial'_\mu - c_2\right] \phi'(x'), \tag{3.130}$$

we can use (3.46) and (3.128) to rewrite

$$\mathcal{A}=\int d^4x\,\phi^*(x)\left[-c_1\hbar^2\partial'^\mu\partial'_\mu-c_2\right]\phi(x). \tag{3.131}$$

But since

$$\partial'_\mu=\Lambda_\mu{}^\nu\partial_\nu,\quad \partial'^\mu=\Lambda^\mu{}_\nu\partial^\nu \tag{3.132}$$

with

$$\Lambda_\mu{}^\nu\equiv g_{\mu\lambda}g^{\nu\kappa}\Lambda^\lambda{}_\kappa, \tag{3.133}$$

we see that

$$\partial'^2\;=\;\partial^2, \tag{3.134}$$

and the transformed action coincides with the original action (3.128).

As in (2.161), we call the integrand of the action a *Lagrangian density*:

$$\mathcal{L}(x)=\phi^*(x)\left[-c_1\hbar^2\partial^\mu\partial_\mu-c_2\right]\phi(x). \tag{3.135}$$

Then the invariance of the action under Lorentz transformations is a direct consequence of the Lagrangian density being a scalar field satisfying the transformation law (3.46):

$$\mathcal{L}'(x')=\mathcal{L}(x), \tag{3.136}$$

which follows directly from the invariance (3.134) and $\phi'(x')=\phi(x)$.

The free-field equation of motion is derived by varying the action (3.128) with respect to the fields $\phi(x),\phi^*(x)$ independently. The independence of these variables is expressed by the functional differentiation rules

$$\begin{aligned}\frac{\delta\phi(x)}{\delta\phi(x')}&=\delta^{(4)}(x-x'),\quad &\frac{\delta\phi^*(x)}{\delta\phi^*(x')}&=\delta^{(4)}(x-x'),\\ \frac{\delta\phi(x)}{\delta\phi^*(x')}&=0, &\frac{\delta\phi^*(x)}{\delta\phi(x')}&=0.\end{aligned} \tag{3.137}$$

Applying these rules to (3.128) we obtain directly

$$\begin{aligned}\frac{\delta\mathcal{A}}{\delta\phi^*(x)}&=\int d^4x'\,\delta^{(4)}(x'-x)(-c_1\hbar^2\partial'^2+c_2)\phi(x')\\ &=(-c_1\hbar^2\partial^2+c_2)\phi(x)=0.\end{aligned} \tag{3.138}$$

Similarly

$$\begin{aligned}\frac{\delta\mathcal{A}}{\delta\phi(x)}&=\int d^4x'\,\phi^*(x')(-c_1\hbar^2\partial'^2+c_2)\delta^{(4)}(x'-x)\\ &=\phi^*(x)(-c_1\hbar^2\overleftarrow{\partial}^2+c_2)=0,\end{aligned} \tag{3.139}$$

where the arrow on top of the last derivative indicates that it acts on the field to the left. The second equation is just the complex conjugate of the previous one.

The field equations (3.138) and (3.139) can be derived directly from the Lagrangian density (3.135) by forming ordinary partial derivatives of $\mathcal{L}$ with respect to all fields and their derivatives. Indeed, a functional derivative of a local action can be expanded in terms of derivatives of the Lagrangian density according to the general rule

$$\frac{\delta \mathcal{A}}{\delta \phi(x)} = \frac{\partial \mathcal{L}(x)}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial \left[\partial_\mu \phi(x)\right]} + \partial_\mu \partial_\nu \frac{\partial \mathcal{L}(x)}{\partial \left[\partial_\mu \partial_\nu \phi(x)\right]} + \dots \,, \tag{3.140}$$

and a similar expansion holds for the derivative with respect to $\phi^*(x)$. These expansions follow directly from the defining relations (3.137). Applying them to the Lagrangian density (3.135), the field equation for $\phi(x)$ is particularly simple:

$$\frac{\delta \mathcal{A}}{\delta \phi^*(x)} = \frac{\partial \mathcal{L}(x)}{\partial \phi^*(x)} = (-c_1 \hbar^2 \partial^2 + c_2)\phi(x) = 0. \tag{3.141}$$

For $\phi^*(x)$, on the other hand, all derivatives written out in (3.140) have to be evaluated to obtain

$$\frac{\delta \mathcal{A}}{\delta \phi(x)} = \frac{\partial \mathcal{L}(x)}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial \left[\partial_\mu \phi(x)\right]} + \partial_\mu \partial_\nu \frac{\partial \mathcal{L}(x)}{\partial \left[\partial_\mu \partial_\nu \phi(x)\right]} = (-c_1 \hbar^2 \partial^2 + c_2)\phi^*(x) = 0. \tag{3.142}$$

The equation

$$\frac{\partial \mathcal{L}(x)}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}(x)}{\partial \partial_\mu \phi(x)} + \partial_\mu \partial_\nu \frac{\partial \mathcal{L}(x)}{\partial \partial_\mu \partial_\nu \phi(x)} + \dots = 0 \tag{3.143}$$

is the Euler-Lagrange equation of a general local field theory. This expression is invariant under partial integrations within the local action $\mathcal{A} = \int d^4x \, \mathcal{L}(x)$. Take for example a Lagrangian density which is equivalent to (3.135) by a partial integration in the action (3.131):

$$\mathcal{L} = c_1 \hbar^2 \partial \phi^*(x) \partial \phi(x) - c_2 \phi^*(x) \phi(x). \tag{3.144}$$

Inserted into (3.143), they produce once more the same field equations.

The field equations (3.141) and (3.142) are solved by the quantum mechanical plane waves (3.34). Moreover, since these equations are of second order in the time derivative, there are two solutions for each spatial momentum, the wave function (3.34), and once more the same wave with the opposite frequency const $e^{i(p^0x^0+\mathbf{px})/\hbar}$. We may reverse the spatial momentum of the latter and use the complex-conjugate pair

$$f_p(x) = \mathcal{N} e^{-ipx/\hbar}, \qquad f_p^*(x) = \mathcal{N} e^{ipx/\hbar}, \tag{3.145}$$

as a complete set of plane-wave solutions. The field equations (3.141) and (3.142) require the four-momenta to satisfy the condition

$$c_1 p^\mu p_\mu - c_2 = 0. \tag{3.146}$$

This has precisely the form of the mass shell relation (3.30) if we choose

$$\frac{c_2}{c_1} = M^2c^2. \tag{3.147}$$

A positive sign of c_1 is necessary for the field fluctuations to be stable. The size can be brought to unity by a multiplicative renormalization of the field. This makes the field normalization different from the nonrelativistic one in the action (3.127).

After this, the mass shell condition fixes the free-field action to the standard form

$$\mathcal{A} = \int d^4x\, \phi^*(x) \left[-\hbar^2\partial^\mu\partial_\mu - M^2c^2\right] \phi(x). \tag{3.148}$$

Since the zeroth component of the four-momenta are fixed in the wave functions (3.145), it is sufficient to label the wave functions (3.145) by their spatial momenta only, using the notation

$$f_{\mathbf{p}}(x) = \mathcal{N}e^{-ipx/\hbar}, \qquad f^*_{\mathbf{p}}(x) = \mathcal{N}e^{ipx/\hbar}. \tag{3.149}$$

It is important to realize that the two sets of solutions (3.149) are independent of each other. They differ in the sign of energy

$$i\partial_0 f_{\mathbf{p}}(x) = p^0 f_{\mathbf{p}}(x), \qquad i\partial_0 f^*_{\mathbf{p}}(x) = -p^0 f^*_{\mathbf{p}}(x). \tag{3.150}$$

For this reason they will be referred to as positive- and negative-frequency wave functions, respectively. In contrast to the nonrelativistic Schrödinger field, a relativistic scalar field $\phi(x)$ contains both frequencies.

The nonrelativistic limit of the action (3.148) is obtained by removing from the positive frequency part of the field $\phi(x)$ a fast trivial oscillating factor corresponding to the rest energy Mc^2, replacing

$$\phi(x) \rightarrow e^{-iMc^2t/\hbar}\frac{1}{\sqrt{2M}}\psi(\mathbf{x},t). \tag{3.151}$$

For a plane wave $f_p(x)$ in (3.145), the field $\psi(\mathbf{x},t)$ becomes $f^\psi_{\mathbf{p}}(\mathbf{x},t) = \mathcal{N}e^{-i(p^0c-Mc^2)t/\hbar}e^{i\mathbf{px}/\hbar}$. In the limit of large c, the first exponential becomes $e^{-i\mathbf{p}^2t/2M}$, such that the field $f^\psi_{\mathbf{p}}(\mathbf{x},t)$ extremizes the nonrelativistic action (3.127). The plane wave $f^*_p(x)$ in (3.145), on the other hand, does not contribute since it yields $\mathcal{N}e^{i(p^0c+Mc^2)t/\hbar}e^{i\mathbf{px}/\hbar}$ which has a temporal prefactor $e^{2iMc^2t/\hbar}$. This oscillates infinitely rapidly for $c \rightarrow \infty$ and is therefore equivalent to zero by the Riemann-Lebesgue Lemma.[5]

The appearance of the constants $\hbar$ and c in all future formulas can be avoided if we work from now on with new fundamental units l_0, m_0, t_0, E_0 different from the ordinary cgs units. They are chosen to give $\hbar$ and c the value 1. Expressed in terms of the conventional length, time, mass, and energy, these new *natural units* are given by

---

[5] This statement holds in the sense of distribtions. Any integral over an infinitely rapidly oscillating function multiplied by a smooth function yields zero.

$$
\begin{aligned}
l_0 &= \frac{\hbar}{Mc}, \qquad t_0 = \frac{\hbar}{Mc^2}, && (3.152)\\
m_0 &= M, \qquad E_0 = Mc^2. && (3.153)
\end{aligned}
$$

If, for example, the particle is a proton with mass m_p, these units are

$$
\begin{aligned}
l_0 &= 2.103138 \times 10^{-11}\text{cm} && (3.154)\\
&= \text{Compton wavelength of proton,}\\
t_0 &= l_0/c = 7.0153141 \times 10^{-22}\text{sec} && (3.155)\\
&= \text{time it takes light to cross the Compton wavelength,}\\
m_0 &= m_p = 1.6726141 \times 10^{-24}\text{g}, && (3.156)\\
E_0 &= 938.2592\,\text{MeV}. && (3.157)
\end{aligned}
$$

For any other mass, they can easily be rescaled.

With these natural units we can drop c and $\hbar$ in all formulas and write the action simply as

$$\mathcal{A} = \int d^4x\, \phi^*(x)(-\partial^2 - M^2)\phi(x). \qquad (3.158)$$

Actually, since we are dealing with relativistic particles there is no fundamental reason to assume $\phi(x)$ to be a complex field. In the nonrelativistic theory this was necessary in order to construct a term linear in the time derivative

$$\int dt\, \phi^* i\partial_t \phi. \qquad (3.159)$$

For a real field $\phi(x)$ this would have been a pure surface term and thus not influenced the dynamics of the system. For second-order time derivatives as in (3.158) this is no longer necessary.

Thus we shall also study the real scalar field with an action

$$\mathcal{A} = \frac{1}{2}\int d^4x\, \phi(x)(-\partial^2 - M^2)\phi(x). \qquad (3.160)$$

In this case it is customary to use a prefactor 1/2 to normalize the field.

The Lagrange density of the complex scalar field may be taken either as

$$\mathcal{L}(x) = \phi^*(x)(-\partial^2 - M^2)\phi(x), \qquad (3.161)$$

or

$$\mathcal{L}(x) = \frac{1}{2}[\partial\phi^*(x)\partial\phi(x) - M^2\phi^*(x)\phi(x)], \qquad (3.162)$$

with an obvious modification for real fields $\phi(x)$. The surface term by which the associated actions differ from one another after a partial integration does not change the Euler-Lagrange equation (3.143). From either Lagrangian, we obtain the *Klein-Gordon equation*

$$(-\partial^2 - M^2)\phi(x) = 0. \tag{3.163}$$

For a complex field, there exists an important local conservation law, which generalizes Eq. (1.30) of Schrödinger theory to relativistic fields. We define the four-vector of probability current density

$$j_\mu(x) = i\phi^* \overleftrightarrow{\partial}_\mu \phi, \tag{3.164}$$

which described the probablity flow of the Klein-Gordon particle. It is easy to verify that due to (3.163), this satisfies *current conservation law*

$$\partial_\mu j^\mu(x) = 0. \tag{3.165}$$

This conservation law will permit us in Chapter 16 to couple electromagnetism to the field and identify $j^\mu(x)$ as the electromagnetic current (if we choose natural units in which the electric charge e is equal to unity).

The deeper reason for the existence of a conserved current will be understood in Subsec. 6.11.1, where we shall see that it is intimately connected with an invariance of the action (3.158) of a free complex scalar field under arbitrary changes of the phase of the field

$$\phi(x) \to e^{-i\alpha}\phi(x). \tag{3.166}$$

It is this invariance which gives rise to a conserved current density [see (6.241), also (16.67)].

The zeroth component of $j^\mu(x)$ the the probability current density

$$\rho(x) = j^0(x). \tag{3.167}$$

describes the charge density. The spatial integral over $\rho(x)$ is the total probability equal to the total charge in natural units:

$$Q(t) = \int d^3x\, j^0(x). \tag{3.168}$$

Because of the local conservation law (3.165), the charge does not depend on time. This is seen by rewriting

$$\dot{Q}(t) = \int d^3x\, \partial_0 j^0(x) = \int d^3x\, \partial_\mu j^\mu(x) - \int d^3x\, \partial_i j^i(x) = -\int d^3x\, \partial_i j^i(x) \tag{3.169}$$

and applying to the right-hand side Gauss theorem as in (1.32), assuming the currents to vanish at spatial infinity.

By removing from the positive-frequency solutions of the Klein-Gordon field $\phi(x)$ the fast oscillation as in (3.151), we can take the nonrelativistic limit and find that the nonrelativistic limit of the spatial part of the current density (3.164) satisfies the local conservation law (1.30) of Schrödinger theory.

Since the current conservation law (3.165) is the direct relativistic generalization of the nonrelativistic probability conservation law (1.30), it is suggestive to define the matrix elements of the charge $Q(t)$ as the scalar product between relativistic wave functions such as the plane waves (3.145). For any two of them, we define

$$(f_{\mathbf{p}'}, f_{\mathbf{p}})_t \equiv \int d^3x \, f^*_{\mathbf{p}'}(\mathbf{x}, t) i \overset{\leftrightarrow}{\partial_0} f_{\mathbf{p}}(\mathbf{x}, t). \tag{3.170}$$

The scalar poduct is formed as a spatial integral at any fixed time as emphasized by the subscript t, but it is time-independent because of charge conservation. Analogous scalar products exist between positive- and negative-frequency solutions $f_{\mathbf{p}}(t)$ and $f^*_{\mathbf{p}}(t)$, and between two negative-frequency solutions $f^*_{\mathbf{p}}(t)$. Both sets of wave functions $f_{\mathbf{p}}(x)$ and $f^*_{\mathbf{p}}(x)$ are needed to span the space of all solutions of the Klein-Gordon equation. Within the scalar product (3.170), we choose to normalize the plane wave functions so that they satisfy the orthogonality relations

$$(f_{\mathbf{p}'}, f_{\mathbf{p}})_t = \delta_{\mathbf{p}',\mathbf{p}}, \quad (f^*_{\mathbf{p}'}, f^*_{\mathbf{p}})_t = -\delta_{\mathbf{p}',\mathbf{p}}, \quad (f^*_{\mathbf{p}'}, f_{\mathbf{p}})_t = 0. \tag{3.171}$$

The spatial integrals ensure the spatial momenta to be equal or opposite to each other. Then the energies p^0 are equal to each other, so that the time derivative in the scalar products produces either zero (between $f_{\mathbf{p}}(t)$ and $f^*_{-\mathbf{p}}(t)$, or a nonzero between equal wave functions. In a finite volume V, these values are the norms of the wave functions $f_{\mathbf{p}}(\mathbf{x}, t)$ and $f^*_{\mathbf{p}}(\mathbf{x}, t)$. They coincide with the matrix elements of the charge (3.168), if the appropriate plane wave is inserted for the field $\phi(x)$ in (3.164). The charge of the plane waves $f^*_{\mathbf{p}}(\mathbf{x}, t)$ is negative, implying that the scalar product is not positive definite. Historically, this has prevented the Klein-Gordon theory from being a direct generalization of Schrödinger theory to relativistic particles; rightfully so, as we shall see in Chapter 5.

In a finite total spatial volume V, the normalized versions of the wave functions (3.149) are then

$$f_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{2Vp^0}} e^{-ipx}, \qquad f^*_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{2Vp^0}} e^{ipx}. \tag{3.172}$$

where p^0 is the particle energy $p^0 = \omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2}$. The norms are ±1.

In an infinite volume, a convenient normalization is

$$\mathrm{f}_{\mathbf{p}}(\mathbf{x}, t) = e^{-ipx}, \qquad \mathrm{f}^*_{\mathbf{p}}(\mathbf{x}, t) = e^{ipx}, \tag{3.173}$$

and the orthogonality relations become

$$\begin{aligned}
(\mathrm{f}_{\mathbf{p}'}, \mathrm{f}_{\mathbf{p}})_t &= 2p^0 \, \delta^{(3)}(\mathbf{p}' - \mathbf{p}), \\
(\mathrm{f}^*_{\mathbf{p}'}, \mathrm{f}^*_{\mathbf{p}})_t &= -2p^0 \, \delta^{(3)}(\mathbf{p}' - \mathbf{p}), \\
(\mathrm{f}^*_{\mathbf{p}'}, \mathrm{f}_{\mathbf{p}})_t &= 0,
\end{aligned} \tag{3.174}$$

where $\bar{\delta}^{(3)}(\mathbf{p}'-\mathbf{p}) = (2\pi)^3\delta^{(3)}(\mathbf{p}'-\mathbf{p})$ as defined in Eq. (1.122). The convenience in having a factor $2p^0$ accompany the $\bar{\delta}$-function is that this combination has pleasant transformation properties under the Lorentz group. It gives unity when integrated over the volume element in momentum space

$$\int \frac{d^3p}{(2\pi)^3 2p^0}. \tag{3.175}$$

This, however, can be rewritten as

$$\int \frac{d^4p}{(2\pi)^3}\Theta(p^0)\delta(p^2-M^2), \tag{3.176}$$

which is obviously Lorentz invariant.

3.5 OTHER SYMMETRIES OF SCALAR ACTION

The actions (3.158) and (3.160) of a real or complex scalar field are invariant under more than just the Lorentz group.

3.5.1 Translations

First, the actions are invariant under space as well as time translations of the coordinate system

$$x'^\mu = x^\mu + a^\mu. \tag{3.177}$$

Recall that under Lorentz transformations, a scalar field at the same spacetime point remains unchanged by the change of coordinates

$$\phi(x) \xrightarrow{\Lambda} \phi'_\Lambda(x) = \phi(\Lambda^{-1}x). \tag{3.178}$$

The same is true for translations:

$$\phi(x) \xrightarrow{a} \phi'_a(x) = \phi(x-a). \tag{3.179}$$

Inserting this into the Lagrangian density (3.161), we see that it transforms like a scalar field

$$\mathcal{L}'(x) = \mathcal{L}(x-a). \tag{3.180}$$

Together with the the trivial translational invariance of the volume integral, the action is indeed invariant.
The combinations of Lorentz transformations and translations

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu \tag{3.181}$$

form a group called the *inhomogeneous Lorentz group* or *Poincaré group*. Under it, the scalar field transforms as

$$\phi(x) \longrightarrow \phi'(x) = \phi(\Lambda^{-1}(x-a)). \tag{3.182}$$

Thus, a free scalar field theory is not only Lorentz-invariant but also Poincaré-invariant. This holds also for real and complex scalar fields $\phi(x)$.

Translations can be generated by a differential operator in just the same way as Lorentz transformations in Eq. (3.116). Obviously we can write the translation (3.179) as

$$\phi(x) \longrightarrow \phi'_a(x) = \phi(x-a) = \hat{D}(a)\phi(x) \equiv e^{ia^\mu \hat{p}_\mu/\hbar}\phi(x), \tag{3.183}$$

where $\hat{p}_\mu = i\hbar\partial_\mu$ is the differential operator of momentum (3.32). This is proved by applying Lie's expansion formula (3.99) to the coordinates x^μ:

$$e^{ia^\mu \hat{p}_\mu/\hbar} x^\lambda e^{ia^\mu \hat{p}_\mu/\hbar} = e^{-a^\mu \partial_\mu} x^\lambda e^{a^\mu \partial_\mu} = x^\lambda - a^\lambda, \tag{3.184}$$

Poincaré transformations are then obtained from operations

$$\phi(x) \longrightarrow \phi'_a(x) = \phi(\Lambda^{-1}(x-a)) = \hat{D}(a)\hat{D}(\Lambda)\phi(x) \equiv e^{ia^\mu \hat{p}_\mu/\hbar} e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}}\phi(x), \tag{3.185}$$

with the parameters $\omega_{\mu\nu}$ specified in (3.66), (3.67). This follows from the behavior of the coordinate vector:

$$e^{ia^\mu \hat{p}_\mu/\hbar} e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} x^\lambda e^{i\frac{1}{2}\omega_{\mu\nu}\hat{L}^{\mu\nu}} e^{-ia^\mu \hat{p}_\mu/\hbar} x^\lambda = (\Lambda^{-1})^\mu{}_\nu (x-a)^\nu, \tag{3.186}$$

thus extending (3.112) to the Poincaré group. The last equation states in a global way the vector properties of x^μ under Poincaré transformations.

3.5.2 Space Inversion

Second, the scalar actions (3.158) and (3.160) are invariant under the operation of *space inversion* [see (3.117)], under which the coordinates go into

$$x \xrightarrow{P} x'_P = \tilde{x} \equiv (x^0, -x^i), \tag{3.187}$$

whereas the scalar field is transformed as follows

$$\phi(x) \xrightarrow{P} \phi'_P(x) = \phi(\tilde{x}). \tag{3.188}$$

Note that this transformation behavior is not the only possible one. Since the parity operation is not related continuously to the identity, there is no reason why the field $\phi(x)$ should go into itself as it does for the continuous group of Lorentz transformations. The parity operation forms, together with the unit element, a group called the *group of space reflections*. The group multiplication table reads as follows:

	1	P
1	1	P
P	P	1

(3.189)

The only requirement which the transformation of the field must satisfy is to be consistent with the group multiplication law in the table. This is assured if the successive application of two parity operations, which is the identity operation, leads back to the original field (*cyclicity* of order 2). It is therefore possible to choose any transformation law

$$\phi(x) \xrightarrow{P} \phi'_P(x) = \eta_P \phi(\tilde{x}), \tag{3.190}$$

as long as η_P satisfies $\eta_P^2 = 1$. This allows for two solutions, the above trivial one in (3.190) with $\eta_P = 1$ and the alternating one with $\eta_P = -1$, i.e.,

$$\eta_P = \pm 1. \tag{3.191}$$

Thus the scalar field could also pick up a negative sign upon space reflection.

If the interactions which generate a particle are invariant under the parity operation, the value of η_P is a characteristic property of the particle. It is called the *intrinsic parity* of the particle. States with positive or negative intrinsic parities are familiar in quantum mechanics where they appear as bound states with even or odd orbital angular momentum, respectively. Only a particle with $\eta_P = 1$ is called a proper *scalar particle*, while $\eta_P = -1$ is called a *pseudoscalar particle*.

The most important fundamental particles of odd parity are the π-mesons which are the source of the long-range part of nuclear interactions. The pseudoscalar nature is most simply seen in the decay of π^0 into two photons, which is the main reason for the finite lifetime $\tau = (8.4 \pm 0.6) \times 10^{-17}$sec of this particle (branching ratio of two-photon with respect to all decay channels is 98.798%). In the rest frame of the pion, the two final photons emerge in opposite directions and polarized parallel to each other. Under a space inversion, the two-photon state is transformed into itself, but with reversed polarization directions. This corresponds to a negative parity.

The negative parity of a charged pion π^-, whose lifetime is much longer [$\tau = (2.6030 \pm 0.0024) \times 10^{-8}$sec], can be deduced from the existence of the absorption of a π^--meson at rest by a deuteron. The deuteron is a bound state of a neutron and a proton in an s-wave with parallel spins, so that the total angular momentum of a deuteron at rest is $J = 1$. For an s-wave, the parity of the orbital wave function is positive. An additional pion at rest does not change J. The final state consists of two neutrons flying apart in opposite directions. By the Pauli principle, their wave function has to be antisymmetric. Thus it can only be in spin-singlet states for even orbital angular momenta l, or in spin-triplet states for odd l. Since the final total angular momentum must be $J = 1$, only the spin-triplet $l = 1$ state is allowed. This, however, has a negative parity, which can only be caused by the additional π^--meson being a pseudoscalar. Note that the intrinsic parities of proton and neutron do not matter in this argument since these particles are present before and after the absorption process.

If particles with definite intrinsic parity interact with each other and the interactions are invariant under space reflections, the intrinsic parity supplies characteristic selection rules in scattering and decay processes. In quantum mechanics for example, decays of atomic states in the dipole approximation have to change the parity of the state since the dipole operator itself has a negative parity.

3.5.3 Time Reversal

As a second extension of the Lorentz invariance of the scalar actions (3.158), (3.160) we can reverse the sign of the time axis via the time reversal transformation

$$x \xrightarrow{T} x'_T = -\tilde{x} \tag{3.192}$$

which has the same multiplication table as the parity transformation:

	1	T
1	1	T
T	T	1

(3.193)

The field transforms like

$$\phi(x) \xrightarrow{T} \phi'_T(x) = \eta_T \phi(x_T), \tag{3.194}$$

where again

$$\eta_T = \pm 1. \tag{3.195}$$

Note that this transformation law holds for both real and complex fields. The field transformation law (3.194) should not be confused with the corresponding transformation law of wave functions. In order to clarify this point consider nonrelativistic Schrödinger theory. There, given a solution $\psi(\mathbf{x}, t)$ of the free-particle Schrödinger equation

$$\left(i\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2\right)\psi(\mathbf{x}, t) = 0, \tag{3.196}$$

the wave function $\psi^*(\mathbf{x}, -t)$ is also a solution with the same energy. The presence of only a single time derivative necessitates the complex conjugation. A plane-wave solution of momentum $\mathbf{p}$

$$\psi_{\mathbf{p}}(\mathbf{x}, t) = e^{-iEt/\hbar + i\mathbf{p}\mathbf{x}/\hbar}, \tag{3.197}$$

transforms like

$$\psi_{\mathbf{p}}(\mathbf{x}, t) \xrightarrow{T} \psi'_{\mathbf{p}\,T}(\mathbf{x}, t) = \eta_T \psi^*_{\mathbf{p}}(\mathbf{x}, -t). \tag{3.198}$$

This satisfies the Schrödinger equation

$$\left(i\partial_t + \frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2\right)\psi'_{\mathbf{p}\,T}(\mathbf{x}, t) = 0, \tag{3.199}$$

From (3.197) we see that the right-hand side is equal to

$$\eta_T \psi_{-\mathbf{p}}(\mathbf{x}, t). \tag{3.200}$$

The particle momentum in the transformed wave function is reversed — the particle runs *backwards in time*.

Since the transformation law (3.198) involves complex conjugation, scalar products between two arbitrary wave functions, $\langle\psi_2(t)|\psi_1(t)\rangle = \int d^3x\,\psi_2^*(\mathbf{x},t)\psi_1(\mathbf{x},t)$ go over into their complex conjugates at the negative time:

$$\langle\psi_2(t)|\psi_1(t)\rangle \xrightarrow{T} {}_T\langle\psi_2'(t)|\psi_1'(t)\rangle_T = \langle\psi_2(-t)|\psi_1(-t)\rangle^*.\langle\psi_1(-t)|\psi_2(-t)\rangle. \tag{3.201}$$

This property guarantees the preservation of probabilities under this transformation. In general, any transformation which carries all scalar products into their hermitian conjugates is referred to as *antiunitary*. The antiunitarity implies that the time reversal operation is necessarily *antilinear*. A tranformation is antilinear if the coefficients of a linear combination of wave functions go over into their complex conjugates.

At the level of the Schrödinger differential operators, the antiunitarity produces a sign reversal in the transformation properties of energy and momentum. The defining representation

$$T^{-1}tT = -t, \qquad T^{-1}\mathbf{x}T = \mathbf{x}, \tag{3.202}$$

implies that

$$T^{-1}i\partial_t T = -i\partial_t, \qquad T^{-1}i\partial_{\mathbf{x}}T = i\partial_{\mathbf{x}}. \tag{3.203}$$

The antiunitary representation of this operation is

$$\mathcal{T}^{-1}i\partial_t\mathcal{T} = i\partial_t, \qquad \mathcal{T}^{-1}i\partial_{\mathbf{x}}\mathcal{T} = -i\partial_{\mathbf{x}}. \tag{3.204}$$

It leaves the energy invariant, while reversing the direction of the momentum:

$$E \xrightarrow{T} E, \qquad \mathbf{p} \xrightarrow{T} -\mathbf{p}. \tag{3.205}$$

Thus particles keep their positive energy but run backwards in time. A unitary representation would have the opposite effect and produce a state which cannot be found in nature.

In contrast to the wave functions, the *Schrödinger field operator*, which was the result of second quantization in Chapter 2, transforms under time reversal like

$$\hat\psi(\mathbf{x},t) \xrightarrow{T} \hat\psi_T'(\mathbf{x},t) = \eta_T\hat\psi(\mathbf{x},-t). \tag{3.206}$$

At the operator level, the effects of complex conjugation are brought about by the antilinearity of the time reversal operator $\mathcal{T}$ in the second-quantized Hilbert space. In fact, the transformation law (3.198) for the wave functions can be derived from (3.206). In terms of $\mathcal{T}$, the transformation (3.206) reads

$$\hat\psi(\mathbf{x},t) \xrightarrow{T} \mathcal{T}^{-1}\hat\psi(\mathbf{x},t)\mathcal{T} = \eta_T\hat\psi(\mathbf{x},-t). \tag{3.207}$$

Expanding the field operator terms of creation and annihilation operators as in Eq. (2.216),

$$\hat\psi(\mathbf{x},t) = \int d^3p\,\psi_{\mathbf{p}}(\mathbf{x},t)\,\hat a_{\mathbf{p}}, \tag{3.208}$$

and using the antilinearity of $\mathcal{T}$, we obtain

$$\mathcal{T}^{-1}\hat{\psi}(\mathbf{x},t)\mathcal{T} = \int d^3p\, \psi^*_{\mathbf{p}}(\mathbf{x},t)\, \mathcal{T}^{-1}\hat{a}_{\mathbf{p}}\mathcal{T} = \int d^3p\, e^{iEt/\hbar - i\mathbf{p}\mathbf{x}/\hbar}\, \mathcal{T}^{-1}\hat{a}_{\mathbf{p}}\mathcal{T}. \quad (3.209)$$

According to (3.207), the right-hand side has to be equal to

$$\eta_T \int d^3p\, e^{iEt/\hbar + i\mathbf{p}\mathbf{x}/\hbar}\, \hat{a}_{\mathbf{p}}, \quad (3.210)$$

which implies that the annihilation operators transform like

$$\mathcal{T}^{-1}\hat{a}_{\mathbf{p}}\mathcal{T} = \eta_T \hat{a}_{-\mathbf{p}}. \quad (3.211)$$

A particle of momentum $\mathbf{p}$ goes over into a particle of momentum $-\mathbf{p}$, which is the correct transformation law.

Thus, in spite of their contradictory appearance, the two transformation laws (3.198) for wave functions and (3.206) for Schrödinger fields, with the antiunitary operator implementation (3.207) after field quantization, are completely consistent with each other. Thus we need no longer be astonished about the absence of a complex conjugation on the right-hand side of the field transformation law (3.194).

Another feature of the antiunitarity which has to be kept in mind is that the time-reversed field operator does not satisfy the Schrödinger equation of the original field

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}{\partial_{\mathbf{x}}}^2\right)\hat{\psi}(\mathbf{x},t) = 0, \quad (3.212)$$

but

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}{\partial_{\mathbf{x}}}^2\right)^*\hat{\psi}'_T(\mathbf{x},t) = 0. \quad (3.213)$$

This follows immediately by multiplying (3.212) with the operator $\mathcal{T}$ from the left and passing $\mathcal{T}$ on to the right-hand side of the differential operator. The antilinearity causes the complex conjugation of the differential operator in (3.214). This is necessary to produce the correct Schrödinger equation (3.199) for the time-reversed wave functions.

At first sight the field equation appears to be in contradiction with the correspondence principle from which one might expect equations for operators to go directly over into those for classical objects in the limit of small $\hbar$. Properly, however, this limit must be taken on equations for measurable *amplitudes*, not the operators themselves, and these *do* follow the Schrödinger equation.[6] Take for instance the single-particle amplitude of an arbitrary state $|\Psi\rangle$ in the Heisenberg picture $\langle 0|\hat{\psi}(\mathbf{x},t)|\Psi\rangle$, which satisfies

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2M}{\partial_{\mathbf{x}}}^2\right)\langle 0|\hat{\psi}(\mathbf{x},t)|\Psi\rangle = 0. \quad (3.214)$$

---

[6] Recall *Ehrenfest's theorem* for the semiclassical limit of field equations.

For the time-reversed field operator (3.206), the equation is

$$\left(i\hbar\partial_t+\frac{\hbar^2}{2M}{\partial_{\mathbf{x}}}^2\right)^*\langle 0|\hat{\psi}(\mathbf{x},-t)|\Psi\rangle=0. \tag{3.215}$$

The time-reversed amplitude on the right-hand side is the amplitude for the time reversed state $\mathcal{T}|\Psi\rangle$ (since $\langle 0|\mathcal{T}^{-1}=\langle 0|$):

$$\langle 0|\hat{\psi}(\mathbf{x},-t)|\Psi\rangle=\langle 0|\mathcal{T}^{-1}\hat{\psi}(\mathbf{x},t)\mathcal{T}|\Psi\rangle=\langle 0|\hat{\psi}(\mathbf{x},t)\mathcal{T}|\Psi\rangle. \tag{3.216}$$

This obeys the Schrödinger equation

$$\left(i\hbar\partial_t+\frac{\hbar^2}{2M}{\partial_{\mathbf{x}}}^2\right)\langle 0|\hat{\psi}(\mathbf{x},-t)\mathcal{T}|\Psi\rangle, \tag{3.217}$$

as it should.

The operator implementation of the time reversal transformation will be discussed in detail in the Chapter 5 for fields and particles of different spin and the reader is referred to Subsecs. 5.1.6, 5.3.4, 5.4.3, and 5.5.4. An important observation should, however, be made right here: As a consequence of the antiunitarity, the phase factor η_T appearing in the time reversal transformation of a complex field is arbitrary. It cannot be fixed in the usual way by applying the transformations T twice. The antilinearity will change η_T arising in the first transformation into η_T^*, so that the combined phase factor is $\eta_T\eta_T^*=1$. This is fulfilled for *any* phase factor $\eta_T=e^{i\gamma}$, not just ± 1.

Since the phase factor η_T is arbitrary, it may be chosen arbitrarily, for instance

$$\eta_T\equiv 1. \tag{3.218}$$

3.5.4 Charge Conjugation

At the level of a relativistic scalar field $\phi(x)$ there is one more discrete symmetry. We can change $\phi(x)$ into $\phi^*(x)$ without changing the action (3.158). This operation is called *charge conjugation* and denoted by C. Since $C^2=1$, a complex field can transform in two possible ways

$$\phi(x)\xrightarrow{C}\phi'_C(x)=\eta_C\phi^*(x), \tag{3.219}$$

where the phase factor can take the values

$$\eta_C=\pm 1. \tag{3.220}$$

For a real field with the action (3.160), we may simply drop the complex conjugation on the right-hand side of (3.219).

An explanation is necessary for the name of this operation. In Eq. (3.164) we have seen that there exists a conserved current $j^\mu(x)$ which can be used to couple the complex scalar field to electromagnetism. If this is done, $j^\mu(x)$ becomes an electromagnetic current density, and $Q(t) = \int d^3x\, j^0(x)$ the charge of the field system. Now, under the transformation (3.219) this electromagnetic current density changes its sign:

$$j^\mu(x) \xrightarrow{C} j_C^{\mu\prime}(x) = -j^\mu(x), \tag{3.221}$$

Thus the transformation reverses the charge of the field, and this is why the discrete operation C is called charge conjugation.

As we shall discuss later in Chapter 22, electromagnetic and strong interactions are invariant under charge conjugation, implying that the phase factor η_C is a fixed measurable property of the particle, called *charge parity*.

Take for instance the neutral π-meson. As mentioned above, it decays in $(8.4 \pm 0.6) \times 10^{-17}$sec mostly into two photons. Since these are also neutral particles, they have a charge parity on their own. Whatever it is (we shall see in Subsec. 3.7.2 that photons have a negative charge parity η_C), the two-photon state must have a positive charge parity, and this must consequently be the charge parity of the π-meson.

3.6 ELECTROMAGNETIC FIELD

Electromagnetic fields move with light velocity and have no mass term.[7] The fields have two polarization degrees of freedom (right and left polarized for circular polarization) and are described by the usual electromagnetic action. Historically, this was the very first example of a relativistic classical field theory. Thus it could also have served as a guideline for the previous construction of the action (3.160) of a real scalar field $\phi(\mathbf{x})$.

3.6.1 Action and Field Equations

The action may be given in terms of a real auxiliary four-vector potential $A_\mu(x)$ from which the physical electric and magnetic fields can be derived as follows

$$\begin{aligned} E^i &= -(\partial^0 A^i - \partial^i A^0) = -\partial_t A^i - \partial_i A^0, & (3.222)\\ B^i &= -\frac{1}{2}\epsilon_{ijk}(\partial^j A^k - \partial^k A^j) = \frac{1}{2}\epsilon_{ijk}(\partial_j A^k - \partial_k A^j). & (3.223) \end{aligned}$$

It is useful to introduce the so-called *four-curl* of the vector potential, the tensor

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{3.224}$$

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[7] The best upper limit for the mass of the electromagnetic field M_γ deduced under terrestrial conditions, from the shape of the earth's magnetic field, is $M_\gamma < 4 \cdot 10^{-48}$g corresponding to a Compton wavelength $\lambda_\gamma = \hbar/M_\gamma c > 10^{10}$cm, which is larger than the diameter of the sun. Astrophysical considerations ("wisps" in the crab nebula) give $\lambda_\gamma > 10^{16}$cm. If metagalactic magnetic fields could be discovered, the Compton wavelength would be larger than $10^{24} - 10^{25}$cm, quite close to the ultimate limit set by the horizon of the universe$=$ $c\times$ age of the universe $\sim 10^{28}$cm. See G.V. Chibisov, Sov. Phys. Usp. *19*, 624 (1976).

Its six components are directly the electric and magnetic field strengths

$$\begin{aligned} F_{0i} &= -F^{0i} = -\partial^0 A^i + \partial^i A^0 = -\partial_0 A^i - \partial_i A^0 = E^i, && (3.225)\\ F_{ij} &= F^{ij} = \partial^i A^j - \partial^j A^i = -\partial_i A^j + \partial_j A^i = -\epsilon_{ijk} B^k, && (3.226)\end{aligned}$$

or, in a more conventional notation

$$\begin{aligned} \mathbf{E}(x) &= -\frac{1}{c}\dot{\mathbf{A}}(x) - \boldsymbol{\nabla} A^0(x), && (3.227)\\ \mathbf{B}(x) &= \boldsymbol{\nabla}\times\mathbf{A}(x). && (3.228)\end{aligned}$$

For this reason the tensor $F_{\mu\nu}$ is also called the *field tensor*. Note that $F^{\mu\nu}$ is related to the fields B_i and E_i in the same way as the generators $L_{\mu\nu}$ of the Lorentz group were related to L_i and M_i in Eq. (3.63).

The electromagnetic action reads

$$\mathcal{A} = \int d^4x\,\mathcal{L} = \int d^4x\,\frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2) = -\frac{1}{4}\int d^4x\,F_{\mu\nu}F^{\mu\nu}. \tag{3.229}$$

The four-curl $F_{\mu\nu}$ satisfies a so-called *Bianchi identity* for any smooth A_μ:

$$\partial_\mu \tilde{F}^{\mu\nu} = 0, \tag{3.230}$$

where

$$\tilde{F}^{\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\lambda\kappa}F_{\lambda\kappa} \tag{3.231}$$

is the *dual field tensor*, with $\epsilon^{\mu\nu\lambda\kappa}$ being the four-dimensional Levi-Civita tensor with $\epsilon_{0123} = 1$. Equation (3.230) can be rewritten as

$$\frac{1}{2}\epsilon^{\mu\nu\lambda\kappa}\partial_\mu F_{\lambda\kappa} = \frac{1}{2}\epsilon^{\mu\nu\lambda\kappa}(\partial_\mu\partial_\lambda - \partial_\lambda\partial_\mu)A_\kappa(x) = 0. \tag{3.232}$$

Multiplying this by another ϵ-tensor and using the tensor identity

$$\begin{aligned} \epsilon_{\mu\nu\lambda\kappa}\epsilon^{\mu\nu'\lambda'\kappa'} &= \delta_\nu{}^{\nu'}\delta_\lambda{}^{\lambda'}\delta_\kappa{}^{\kappa'} + \delta_\nu{}^{\lambda'}\delta_\lambda{}^{\kappa'}\delta_\kappa{}^{\nu'} + \delta_\nu{}^{\kappa'}\delta_\lambda{}^{\nu'}\delta_\kappa{}^{\lambda'}\\ &\quad -\delta_\nu{}^{\lambda'}\delta_\lambda{}^{\nu'}\delta_\kappa{}^{\kappa'} - \delta_\nu{}^{\nu'}\delta_\lambda{}^{\kappa'}\delta_\kappa{}^{\lambda'} - \delta_\nu{}^{\kappa'}\delta_\lambda{}^{\lambda'}\delta_\kappa{}^{\nu'}, && (3.233)\end{aligned}$$

we obtain the integrability condition of *Schwarz' lemma*, according to which the derivatives of an integrable function commute:

$$(\partial_\mu\partial_\nu - \partial_\nu\partial_\mu)A_\lambda(x) = 0. \tag{3.234}$$

The equations of motion which extremize the action are

$$\frac{\delta\mathcal{A}}{\delta A^\mu(x)} = -\partial_\mu\frac{\partial\mathcal{L}(x)}{\partial[\partial_\mu A_\nu(x)]} = \frac{1}{2}\partial_\mu F^{\mu\nu}(x) = 0, \tag{3.235}$$

or more explicitly

$$(g^{\mu\nu}\partial^2 - \partial^\mu\partial^\nu)A_\nu(x) = 0. \tag{3.236}$$

Separating the equations (3.230) and (3.235) into space and time components they are seen to coincide with the four Maxwell's equations in empty space:

$$\partial_\mu \tilde{F}^{\mu\nu} = 0: \quad \boldsymbol{\nabla}\cdot\mathbf{B} = 0, \quad \boldsymbol{\nabla}\times\mathbf{E} + \partial_t\mathbf{B} = 0, \tag{3.237}$$

$$\partial_\mu F^{\mu\nu} = 0: \quad \boldsymbol{\nabla}\cdot\mathbf{E} = 0, \quad \boldsymbol{\nabla}\times\mathbf{B} - \partial_t\mathbf{E} = 0. \tag{3.238}$$

The first equation in (3.237) states that there can be no magnetic monopoles. The second equation is *Faraday's law* of induction. The first equation in (3.238) is *Coulomb's law* in the absence of charges, the second is *Ampère's law* in the absence of currents (including, however, Maxwell's displacement current caused by the time derivative of the electric field).

In terms of the vector field $A^\mu(x)$, the action reads explicitly

$$\begin{aligned}\mathcal{A} = \int d^4x\, \mathcal{L}(x) &= -\frac{1}{2}\int d^4x\, [\partial^\mu A^\nu(x)\partial_\mu A_\nu(x) - \partial^\nu A_\nu(x)\partial^\mu A_\mu(x)] \\ &= \frac{1}{2}\int d^4x\; A_\mu(x)(g^{\mu\nu}\partial^2 - \partial^\mu\partial^\nu)A_\nu(x).\end{aligned} \tag{3.239}$$

The latter form is very similar to the scalar action (3.160). The first piece is the same as in (3.160) for each of the spatial components A^1, A^2, A^3. The time component A^0, however, appears with an opposite sign. A field with this property is called a *ghost field*. When trying to quantize such a field the associated particle states turn out to have a negative norm. If the theory is to be physically consistent, such states must never appear in any scattering process. The second term $\partial^\nu A_\nu \partial^\mu A_\mu$ in the action (3.239) is novel with respect to the scalar case. It exists here as an additional possible Lorentz invariant since A_μ is a vector field under Lorentz transformations.

3.6.2 Gauge Invariance

The field tensor (3.224) is invariant under local gauge transformations

$$A_\mu(x) \longrightarrow A'_\mu(x) = A_\mu(x) + \partial_\mu\Lambda(x), \tag{3.240}$$

where $\Lambda(x)$ is any smooth field which satisfies the integrability condition

$$(\partial_\mu\partial_\nu - \partial_\nu\partial_\mu)\Lambda(x) = 0. \tag{3.241}$$

Gauge invariance implies that one scalar field degree of freedom in $A^\mu(x)$ does not contribute to the physically observable electromagnetic fields $\mathbf{E}(x)$ and $\mathbf{B}(x)$. This degree of freedom can be removed by *fixing a gauge*. One way to do that is to require the vector potential to satify the *Lorentz gauge condition* of having no four-divergence:

$$\partial_\mu A^\mu(x) = 0. \tag{3.242}$$

For a vector field satisfying this condition, the field equations (3.236) decouple end become simply four massless Klein-Gordon equations:

$$-\,\partial^2 A_\nu(x) = 0. \tag{3.243}$$

If a vector potential $A^\mu(x)$ does not satisfy this condition, one may always perform a gauge transformation (3.240) to a new field $A'^\mu(x)$ that has no four divergence. We merely have to choose a gauge function $\Lambda(x)$ solving differential equation

$$-\partial^2\Lambda(x) = \partial_\mu A^\mu(x), \tag{3.244}$$

and $A'^\mu(x)$ will satisfy $\partial_\mu A'^\mu(x) = 0$.

There are infinitely many solutions to equation (3.244). Given one solution $\Lambda(x)$ which leads to the Lorentz gauge, one can add any solution of the homogenous Klein-Gordon equation without changing the four-divergence of $A^\mu(x)$. The associated gauge transformations

$$A_\mu(x) \longrightarrow A_\mu(x) + \partial_\mu\Lambda'(x), \qquad \partial^2\Lambda'(x) = 0, \tag{3.245}$$

are called *restricted gauge transformations* or *gauge tansformation of the second kind.* If a vector potential $A^\mu(x)$ in the Lorentz gauge solves the field equations (3.236), the gauge tranformations of the second kind can be used to remove the spatial divergence $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},\mathbf{t})$. Under (3.245), the components $A^0(\mathbf{x},t)$ and $\mathbf{A}(\mathbf{x},t)$ go over into

$$\begin{array}{rcl} A^0(x) & \rightarrow & A'^0(\mathbf{x},t) = A^0(\mathbf{x},t) + \partial_0\Lambda'(\mathbf{x},t), \\ \mathbf{A}(x) & \rightarrow & \mathbf{A}'(\mathbf{x},t) = \mathbf{A}(\mathbf{x},t) - \boldsymbol{\nabla}\Lambda'(\mathbf{x},t). \end{array} \tag{3.246}$$

Thus, if we choose the gauge function

$$\Lambda'(\mathbf{x},t) = -\int d^3x' \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x}',t), \tag{3.247}$$

then

$$\boldsymbol{\nabla}^2\Lambda'(\mathbf{x},t) = \boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t) \tag{3.248}$$

and the gauge-transformed field $\mathbf{A}'(\mathbf{x},t)$ has no spatial divergence: it is completely transverse:

$$\boldsymbol{\nabla}\cdot\mathbf{A}'(\mathbf{x},t) = \boldsymbol{\nabla}\cdot[\mathbf{A}(\mathbf{x},t) - \boldsymbol{\nabla}\Lambda(\mathbf{x},t)] = 0. \tag{3.249}$$

The condition

$$\boldsymbol{\nabla}\cdot\mathbf{A}'(\mathbf{x},t) = 0 \tag{3.250}$$

is known as the *Coulomb-* or *radiation gauge*.

The solution (3.247) to the differential equation (3.248) is undetermined up to an arbitrary solution $\Lambda'(x)$ of the homogeneous Poisson equation

$$\boldsymbol{\nabla}^2\Lambda'(\mathbf{x},t) = 0. \tag{3.251}$$

Together with the property $\partial^2\Lambda'(\mathbf{x},t) = 0$ from (3.245), one also has

$$\partial_t^2\Lambda'(\mathbf{x},t) = 0. \tag{3.252}$$

This leaves only trivial linear functions $\Lambda'(\mathbf{x},t)$ of $\mathbf{x}$ and t which do not describe propagating waves.

Another possible gauge is obained by removing the zeroth component of the vector potential $A^\mu(x)$ satisfying the field equations (3.236). We form again

$$A'^\mu(x) = A^\mu(x) + \partial^\mu\Lambda(x), \tag{3.253}$$

but now with a gauge function

$$\Lambda(\mathbf{x},t) = -\int^t dt'\, A_0(\mathbf{x},t'). \tag{3.254}$$

Then $A'^\mu(x)$ will satisfy the field equations (3.236), while having the property

$$A'^0(x) = 0. \tag{3.255}$$

This is called the *axial gauge*. The solutions of Eqs. (3.254) are determined up to a trivial constant, so that no more gauge freedom is left comparable to the second type in (3.245).

For free fields, the Coulomb gauge and the axial gauge coincide. This is a consequence of Coulomb's law $\boldsymbol{\nabla}\cdot\mathbf{E}=0$ in Eq. (3.238). By expressing $\mathbf{E}(x)$ explicitly in terms of the spatial and time-like components of the vector potential

$$\mathbf{E}(x) = -\partial_0\mathbf{A}(x) - \boldsymbol{\nabla}A^0(x), \tag{3.256}$$

Coulomb's law reads

$$\boldsymbol{\nabla}^2 A^0(\mathbf{x},t) = -\boldsymbol{\nabla}\cdot\dot{\mathbf{A}}(\mathbf{x},t). \tag{3.257}$$

This shows that if $\boldsymbol{\nabla}\cdot\mathbf{A}(x)=0$, also $A^0(x)=0$, and vice versa.

The differential equation (3.257) can be integrated to

$$A^0(\mathbf{x},t) = \frac{1}{4\pi}\int d^3x'\frac{1}{|\mathbf{x}'-\mathbf{x}|}\left(\boldsymbol{\nabla}\cdot\dot{\mathbf{A}}\right)(\mathbf{x}',t). \tag{3.258}$$

In an infinite volume with asymptotically vanishing fields there is no freedom of adding to the left-hand side a notrivial solution of the homogenous Poisson equation

$$\boldsymbol{\nabla}^2 A^0(\mathbf{x},t) = 0, \tag{3.259}$$

which in principle would be possible.

In the presence of charges, Coulomb's law will have a source term and read [see Eq. (10.50)]

$$\boldsymbol{\nabla}\cdot\mathbf{E}(\mathbf{x},t) = \rho(\mathbf{x},t). \tag{3.260}$$

where $\rho(\mathbf{x},t)$ is the electric charge density. In this case the vanishing of $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)$ no longer implies $A^0(\mathbf{x},t)\equiv 0$. Then one has the possibility of choosing $\Lambda(\mathbf{x},t)$ either to satisfy the Coulomb gauge

$$\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t) \equiv 0, \tag{3.261}$$

or the axial gauge

$$A^0(\mathbf{x},t) \equiv 0. \tag{3.262}$$

Only for free fields the two gauges coincide.

In the presence of charges, the canonical field momenta (5.335) will receive an extra contribution from $\boldsymbol{\nabla} A^0(\mathbf{x},t)$ which is the longitudinal classical electric field caused by the charges [see the discussion after Eq. (10.75)].

3.6.3 Lorentz Transformation Properties of Electromagnetic Fields

The Lorentz transformation properties of the electromagnetic fields were understood a long time ago within classical electrodynamics. They are the origin of the famous *Lorentz force* acting on moving charged particles. The experimentally observed electric and magnetic forces can be derived by going from the laboratory frame with fields $\mathbf{E}$, $\mathbf{B}$ to the reference frame of the moving particle with fields $\mathbf{E}'$, $\mathbf{B}'$ and transforming

$$\begin{aligned} \mathbf{E}_{\|}{}' &= \mathbf{E}_{\|}\,, \quad \mathbf{E}_{\perp}{}' = \gamma\left(\mathbf{E}_{\perp} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right), \\ \mathbf{B}_{\|}{}' &= \mathbf{B}_{\|}\,, \quad \mathbf{B}_{\perp}{}' = \gamma\left(\mathbf{B}_{\perp} - \frac{\mathbf{v}}{c}\times\mathbf{E}\right), \end{aligned} \tag{3.263}$$

with $\mathbf{v}$ being the velocity of the particle and $\gamma \equiv 1/\sqrt{1-v^2/c^2}$ the Einstein parameter (3.16). The transformed fields exert the observed electric and magnetic forces $e\mathbf{E}' + g\mathbf{B}'$. The subscripts $\|$ and $\perp$ indicate projections of the fields parallel and orthogonal to $\mathbf{v}$. From this transformation one may *derive* the transformation law of the vector field A_μ under Lorentz transformations. Let the frame in which the moving particle is at rest be related to the laboratory frame by

$$x' = B_{\hat{\mathbf{v}}}(v)x, \tag{3.264}$$

where $B_{\hat{\mathbf{v}}}(v)$ is a boost in $\mathbf{v}$-direction with a rapidity

$$\cosh\zeta = \gamma, \quad \sinh\zeta = \gamma\frac{v}{c}, \quad \tanh\zeta = \frac{v}{c}. \tag{3.265}$$

Then the transformation law (3.263) is equivalent to

$$A'^{\mu}(x') = B_{\hat{\mathbf{v}}}(v)^{\mu}{}_{\nu}A^{\nu}(x), \tag{3.266}$$

apart from an arbitrary gauge transformation. An analogous transformation law holds for rotations, so that the transformations (3.263) and their rotated forms correspond to the Lorentz tansformations

$$A'^{\mu}(x') = \Lambda^{\mu}{}_{\nu}A^{\nu}(x), \tag{3.267}$$

plus possible gauge transformations. In the notation (3.47), we write the transformation law as

$$A^\mu(x) \xrightarrow{\Lambda} A'_\Lambda{}^\mu(x) = \Lambda^\mu{}_\nu A^\nu(\Lambda^{-1}x). \tag{3.268}$$

By analogy with Eq. (3.116) for the scalar field, and recalling (3.65), this transformation can be generated as follows:

$$A^\mu(x) \xrightarrow{\Lambda} A'^\mu(x) = \hat{D}(\Lambda)\Lambda^\mu{}_\nu A^\nu(x) \equiv e^{-i\frac{1}{2}\omega_{\lambda\kappa}\hat{J}^{\lambda\kappa}} A^\mu(x), \tag{3.269}$$

with the parameters $\omega_{\mu\nu}$ specified in (3.66), (3.67), and

$$\hat{J}^{\lambda\kappa} \equiv L^{\lambda\kappa} \times \hat{1} + 1 \times \hat{L}^{\lambda\kappa} \tag{3.270}$$

being the generators of Lorentz transformations of both the vector index and spacetime argument The former are generated by the 4×4 matrices $L_{\mu\nu}$ of Eq. (3.61), the latter by the differential operators (3.90). The combined generators (3.270) are called the generators of the *total four-dimensional angular momentum*. The two generators on the right-hand side of Eq. (3.270) on different spaces, transforming once the vector index and once the spacetime coordinate x. One therefore writes often shorter and somewhat sloppily

$$\hat{J}^{\mu\nu} \equiv L^{\mu\nu} + \hat{L}^{\mu\nu}, \tag{3.271}$$

with the tacit understanding that what is meant is the direct sum (3.270) of spin and orbital generators.

Since the two terms in (3.270) act independently on space and spin indices, the operators $\hat{J}^{\lambda\kappa}$ satisfy the same commutation rules as $L^{\lambda\kappa}$ and $\hat{L}^{\lambda\kappa}$:

$$[\hat{J}^{\mu\nu}, \hat{J}^{\lambda\kappa}] = -i(g^{\mu\lambda}\hat{J}^{\nu\kappa} - g^{\mu\kappa}\hat{J}^{\nu\lambda} + g^{\nu\kappa}\hat{J}^{\mu\lambda} - g^{\nu\lambda}\hat{J}^{\mu\kappa}). \tag{3.272}$$

The transformation laws (3.267) and (3.269) differ from those of a scalar field in Eqs. (3.46) and (3.116) in the way discussed above for particles with nonzero intrinsic angular momentum. The field has several components. It points in the same spatial direction before and after the change of coordinates. This is ensured by its components changing in the same way as the coordinates of the point x_μ.

Note that the four-divergence $\partial^\mu A_\mu(x)$ is a scalar field in the sense defined in (3.46). Indeed

$$\partial'^\mu A'_\mu(x') = (\Lambda^\mu{}_\nu \partial^\nu)\Lambda_\mu{}^\lambda A_\lambda(x) = \partial^\nu A_\nu(x). \tag{3.273}$$

For this reason the second term in the action (3.239) is Lorentz-invariant, just as the mass term in (3.160). The invariance of the first term is shown similarly

$$A'^\nu(x')\partial'^2 A'_\nu(x') = \Lambda^\nu{}_\lambda A^\lambda(x)\partial'^2 \Lambda_\nu{}^\kappa A_\kappa(x') = A^\nu(x)\partial'^2 A_\nu(x) = A^\nu(x)\partial^2 A_\nu(x). \tag{3.274}$$

Hence the action (3.239) does not change under Lorentz transformations, as it should.

3.7 OTHER SYMMETRIES OF ELECTROMAGNETIC ACTION

Just as the scalar action, also the electromagnetic action (3.229) is invariant under more symmetry transformations than those of the Lorentz group.

3.7.1 Translations

Under translations (3.177),

$$x'^{\mu} = x^{\mu} + a^{\mu}, \tag{3.275}$$

the vector field transforms like

$$A'^{\mu}(x) = A^{\mu}(x - a). \tag{3.276}$$

The combination of these with Lorentz transformations forms the Poincaré group (3.181),

$$x'^{\mu} = \Lambda^{\mu}{}_{\nu} x^{\nu} + a^{\mu}, \tag{3.277}$$

under which the field $A^{\mu}(x)$ transforms like

$$A'^{\mu}(x) = \Lambda^{\mu}{}_{\nu} A^{\nu}(\Lambda^{-1}(x - a)), \tag{3.278}$$

leaving the action (3.239) invariant.

As in the scalar equation (3.185), we can generate all Poincaré transformations of the vector potential $A^{\mu}(x)$ with the help of differential operators as

$$A^{\mu}(x) \longrightarrow A'^{\mu}(x) = \hat{D}(a)\hat{D}(\Lambda)\Lambda^{\mu}{}_{\nu} A^{\nu}(x) \equiv e^{ia^{\mu}\hat{p}_{\mu}/\hbar} e^{-i\frac{1}{2}\omega_{\lambda\kappa}\hat{J}^{\lambda\kappa}} A^{\mu}(x), \tag{3.279}$$

with the parameters $\omega_{\mu\nu}$ specified in (3.66), (3.67).

3.7.2 Space Inversion, Time Reversal, and Charge Conjugation

Under space inversion, the four-vector $A^{\mu}(x)$ behaves as follows:

$$A^{\mu}(x) \xrightarrow{P} A'^{\mu}_{P}(x) = \tilde{A}^{\mu}(\tilde{x}). \tag{3.280}$$

Under time reversal one has

$$A^{\mu}(x) \xrightarrow{T} A'^{\mu}_{T}(x) = \tilde{A}^{\mu}(-\tilde{x}), \tag{3.281}$$

where

$$\tilde{A}^{\mu} = (A^{0}, -A^{i}). \tag{3.282}$$

In principle, there is the possibility of a vector field $V^{\mu}(x)$ transforming like

$$V^{\mu}(x)(x) \xrightarrow{P} V'^{\mu}_{P}(x) = \eta_{P} \tilde{V}^{\mu}(\tilde{x}), \tag{3.283}$$

with $\eta_P = \pm 1$. For $\eta_P = -1$ the field $V^\mu(x)$ is called an *axial vector field.* The electromagnetic gauge field $A^\mu(x)$, however, is definitely a vector field. This follows from the vector nature of the electric and the axial vector nature of the magnetic field which are observed in the laboratory.

Similarly, the behavior of a physically observable vector field V^μ with respect to time reversal is given by

$$V^\mu(x) \xrightarrow{T} V'^\mu_T(x) = \eta_T \tilde{V}^{\mu *}(x_T) \tag{3.284}$$

with an arbitrary phase factor η_T. If the vector field is real and physically observable, then the only alternatives are $\eta_T = \pm 1$. For the electromagnetic vector potential $A^\mu(x)$, the phase factor η_T is as specified in (3.281) since under time reversal, all spatial currents change their directions whereas the zeroth component stays the same. This reverses the direction of the **B**-field but has no influence on the **E**-field generated by flowing charges.

The complex conjugation on the right-hand side of (3.284) has the same origin as in the transformation law (3.198) for the complex scalar field.

The operation of charge conjugation is performed by exchanging the sign of all charges without changing their direction of flow. Then both **E** and **B** change their directions. Hence

$$A^\mu(x) \xrightarrow{C} A'^\mu_C(x) = -A^\mu(x). \tag{3.285}$$

In general, the vector field could have transformed as

$$A^\mu(x) \xrightarrow{C} A'^\mu_C(x) = \eta_C A^\mu(x) \tag{3.286}$$

with $\eta_C = \pm 1$. The fact that the electromagnetic field has $\eta_C = -1$ means that it is odd under charge conjugation.

3.8 PLANE-WAVE SOLUTIONS OF MAXWELL'S EQUATIONS

The plane-wave solutions of the field equations (3.236) are direct extensions of Eqs. (3.172) and (3.173):

$$f^\mu_{\mathbf{k}}(\mathbf{x}, t) = \frac{1}{\sqrt{2Vk^0}} \epsilon^\mu(\mathbf{k}, \lambda) e^{-ikx}, \qquad f^{\mu *}_{\mathbf{k}} = \frac{1}{\sqrt{2Vk^0}} \epsilon^{\mu *}(\mathbf{k}, \lambda) e^{ikx}, \tag{3.287}$$

or

$$\mathrm{f}^\mu_{\mathbf{k}}(\mathbf{x}, t) = \epsilon^\mu(\mathbf{k}, \lambda) e^{-ikx}, \qquad \mathrm{f}^{\mu *}_{\mathbf{k}} = \epsilon^{\mu *}(\mathbf{k}, \lambda) e^{ikx}, \tag{3.288}$$

with the momentum on the mass shell with $M = 0$, the so-called *light cone.* The momentum-dependent four-vectors $\epsilon^\mu(\mathbf{k}, \lambda)$ specify the polarization of the plane electromagnetic wave. The label λ counts the different polarization states. In the Lorentz gauge, the vector potential must have a vanishing four divergence (3.242), implying the condition

$$k_\mu \epsilon^\mu(\mathbf{k}, \lambda) = 0. \tag{3.289}$$

Being solutions of the wave equations, there is a further restricted gauge freedom (3.245). We may add to the solutions $f^{\mu}_{\mathbf{k}}(\mathbf{x},t)$ or $\mathrm{f}^{\mu}_{\mathbf{k}}(\mathbf{x},t)$ the total gradient of a function $\Lambda(x)$ which is itself a plane wave $\Lambda(x) = e^{-ikx}$ with k^2=0, thus solving also the Klein-Gordon equation. The total gradient adds to the polarization vector a term proportional of the four-momentum k^{μ}:

$$\epsilon^{\mu}(\mathbf{k},\lambda) \to \epsilon'^{\mu}(\mathbf{k},\lambda) = \epsilon^{\mu}(\mathbf{k},\lambda) + k^{\mu}\Lambda(\mathbf{k},\lambda). \tag{3.290}$$

By choosing

$$\Lambda(\mathbf{k},\lambda) = -\frac{1}{\mathbf{k}^2}\mathbf{k}\cdot\boldsymbol{\epsilon}(\mathbf{k},\lambda), \tag{3.291}$$

the spatial part of the polarization vector $\epsilon'^{\mu}(\mathbf{k},\lambda)$ acquires the property

$$\mathbf{k}\cdot\boldsymbol{\epsilon}(\mathbf{k},\lambda) = 0, \tag{3.292}$$

which is the Coulomb gauge (3.250) for the polarization vector.

We can also choose

$$\Lambda(\mathbf{k},\lambda) = -\frac{1}{k^0}\epsilon^0(\mathbf{k},\lambda), \tag{3.293}$$

and $\epsilon'^{\mu}(\mathbf{k},\lambda)$ will satisfy

$$\epsilon^0(\mathbf{k},\lambda) = 0. \tag{3.294}$$

which is the axial gauge (3.255) for the polarization vector. In Section 3.6.2 we showed that for free fields, the two gauges coincide. we see this here explicitly. The Lorentz gauge (3.289) implies for the spatial and time-like components of $\epsilon^0(\mathbf{k},\lambda)$:

$$k^0\epsilon^0(\mathbf{k},\lambda) = \mathbf{k}\cdot\boldsymbol{\epsilon}(\mathbf{k},\lambda), \tag{3.295}$$

so that the two conditions (3.292) and (3.294) are indeed the same.

Since the four-component vectors $\epsilon^0(\mathbf{k},\lambda)$ are restricted by two conditions, only two of them can be independent. These will be labeled by $\lambda = \pm 1$ and are constructed as follows.

Because of the axial property (3.294) we set

$$\epsilon^{\nu}(\mathbf{k},\lambda) \equiv (0, \boldsymbol{\epsilon}(\mathbf{k},\lambda)), \tag{3.296}$$

and impose on the spatial part the Coulomb gauge property (3.292). This equation is solved by two polarization vectors orthogonal to the spatial momentum $\mathbf{k}$. These are defined uniquely by the following consideration. If $\mathbf{k}$ points in the z-direction, then the two vectors $\boldsymbol{\epsilon}(\mathbf{k},\pm 1)$ coincide with the eigenvectors $\boldsymbol{\epsilon}(\pm 1)$ of the 3×3 - matrix L_3 of the rotation group in Eq. (3.50), with eigenvalues ± 1. There are three eigenvectors $\boldsymbol{\epsilon}(\lambda)$ $(\lambda = 1, 0, -1)$ which are determined by the equations

$$L_3\boldsymbol{\epsilon}(\lambda) = \lambda\,\boldsymbol{\epsilon}(\lambda), \qquad \lambda = 1, 0, -1. \tag{3.297}$$

The result is

$$\boldsymbol{\epsilon}(\pm 1) = \mp\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i \\ 0 \end{pmatrix}, \qquad \boldsymbol{\epsilon}(0) = -\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{3.298}$$

The opposite signs of $\boldsymbol{\epsilon}(\pm1)$ are chosen to comply with the so-called Condon-Shortley phase convention to be discussed in detail in Subsection 3.18.3 (see in particular Footnote 22 and Fig. 3.3). They ensure that the 3×3 raising and lowering matrices formed from the 3×3 spatial submatrices of the generators (3.51) and (3.52),

$$L_\pm = L_1 \pm iL_2 = \begin{pmatrix} 0 & 0 & \mp1 \\ 0 & 0 & -i \\ \pm1 & i & 0 \end{pmatrix}, \tag{3.299}$$

have the positive matrix elements:

$$L_+\boldsymbol{\epsilon}(-1) = \sqrt{2}\,\boldsymbol{\epsilon}(0), \qquad L_+\boldsymbol{\epsilon}(0) = \sqrt{2}\,\boldsymbol{\epsilon}(1), \tag{3.300}$$

$$L_-\boldsymbol{\epsilon}(\ 1) = \sqrt{2}\,\boldsymbol{\epsilon}(0), \qquad L_-\boldsymbol{\epsilon}(0) = \sqrt{2}\,\boldsymbol{\epsilon}(-1). \tag{3.301}$$

The vectors $\boldsymbol{\epsilon}(\pm1)$ and $\boldsymbol{\epsilon}(0)$ are the so-called *spherical components* of the three-dimensional unit vectors

$$\boldsymbol{\epsilon}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \boldsymbol{\epsilon}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \boldsymbol{\epsilon}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{3.302}$$

related by

$$\boldsymbol{\epsilon}(\pm1) \equiv \mp\frac{1}{\sqrt{2}}(\boldsymbol{\epsilon}_1 \pm i\boldsymbol{\epsilon}_2), \tag{3.303}$$

Together with the unit vector

$$\boldsymbol{\epsilon}\,(0) = \boldsymbol{\epsilon}_3, \tag{3.304}$$

they form a basis of the unitary spin-1 representation of the rotation group.

In order to obtain the polarization vectors $\boldsymbol{\epsilon}(\mathbf{k},\pm1)$ for momenta in an arbitrary direction, we must rotate $\boldsymbol{\epsilon}(\pm1)$ into the direction $\hat{\mathbf{k}}$. We shall use the rotation matrix[8]

$$R(\theta,\phi) = e^{-i\phi L_3}e^{-i\theta L_2} = \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \tag{3.305}$$

with the spherical angles

$$\theta \in [0,\pi), \qquad \phi \in [0,2\pi), \tag{3.306}$$

to arrive at a momentum direction

$$\hat{\mathbf{k}} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \tag{3.307}$$

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[8] Some authors prefer the matrix $R(\theta,\phi) = e^{-i\phi L_3}e^{-i\theta L_2}e^{i\phi L_3}$.

with the polarization vectors

$$\boldsymbol{\epsilon}\,(\mathbf{k},\pm1) = \mp\frac{1}{\sqrt{2}}\begin{pmatrix} \cos\theta\cos\phi \mp i\sin\phi \\ \cos\theta\sin\phi \pm i\cos\phi \\ -\sin\theta \end{pmatrix}. \tag{3.308}$$

Together with the third vector

$$\boldsymbol{\epsilon}\,(\mathbf{k},0) \equiv \hat{\mathbf{k}}, \tag{3.309}$$

for which there is no electromagnetic plane wave, they form a representation of spin 1 diagonalizing $\mathbf{L}^2$ and the *helicity matrix* $H = \hat{\mathbf{k}}\cdot\mathbf{L}$ the matrices $\mathbf{L}$ from Eq. (3.53). The labels $\lambda = \pm1$ specify the two helicities of a light wave of momentum $\mathbf{k}$. Experimentally, these waves are observed as right and left circularly polarized light.

Since the spatial polarization vectors are orthogonal to the momentum $\mathbf{k}$ they are also referred to as *transverse polarization vectors*, and the Coulomb gauge condition (3.292) as *transverse gauge condition.*

The spatial polarization vectors $\boldsymbol{\epsilon}(\mathbf{k},\lambda)$ are orthonormal:

$$\boldsymbol{\epsilon}^*(\mathbf{k},\lambda)\cdot\boldsymbol{\epsilon}(\mathbf{k},\lambda') = \delta_{\lambda\lambda'}, \qquad \lambda,\ \lambda' = 0,\pm1. \tag{3.310}$$

This property goes over to the four-dimensional polarization vectors (3.296):

$$\epsilon^*_\mu(\mathbf{k},\lambda)\epsilon^\mu(\mathbf{k},\lambda') = -\delta_{\lambda\lambda'}, \qquad \lambda,\ \lambda' = 0,\pm1. \tag{3.311}$$

These vectors have the reflection property

$$\epsilon^\mu\,(-\mathbf{k},\lambda) = \epsilon^\mu\,(\mathbf{k},-\lambda), \tag{3.312}$$

which follows from the fact that $\mathbf{k} \to -\mathbf{k}$ corresponds to $\theta \to \pi - \theta$, $\phi \to \phi + \pi\,(\mathrm{mod}\ 2\pi)$.

One may define scalar products between the solutions by complete analogy with those for the scalar field in Eqs. (3.170), only that those are multiplied with an extra scalar product between polarization vectors:

$$(f_{\mathbf{p}'}, f_{\mathbf{p}})_t \equiv \int d^3x\, f^{\mu *}_{\mathbf{p}'}(\mathbf{x},t) i\, \overleftrightarrow{\partial_0}\, f_{\mu\mathbf{p}}(\mathbf{x},t), \tag{3.313}$$

with obvious definitions between positive- and negative-frequency solutions $f_{\mathbf{p}'}(t)$ and $f^*_{\mathbf{p}'}(t)$, and between two negative-frequency solutions $f^*_{\mathbf{p}'}(t)$.

Being only two vectors in a four-dimensional space, they are certainly incomplete. Their polarization sum is

$$\begin{aligned} P^{\mu\nu}_{\mathrm{phys}}(\mathbf{k}) = \sum_{\lambda=\pm1}\epsilon^{\mu\,T}(\mathbf{k},\lambda)\epsilon^{\nu *}(\mathbf{k},\lambda) &= \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \delta^{ij} - k^ik^j/\mathbf{k}^2 \end{array}\right)^{\mu\nu} \\ &= -g^{\mu\nu} + \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -k^ik^j/\mathbf{k}^2 \end{array}\right)^{\mu\nu}. \end{aligned} \tag{3.314}$$

This is a 4 × 4 projection matrix into the two-dimensional purely spatial subspace transverse to **k**.

The projection is obviously noncovariant since it lends a special significance to the zeroth component of the electromagnetic vector field. To exhibit the noncovariance, it is useful to introduce a fixed timelike unit vector

$$\eta^{\mu} \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{3.315}$$

We also define a purely spacelike unit vector orthogonal to it pointing in the direction of **k**:

$$\bar{k}^{\mu} \equiv \begin{pmatrix} 0 \\ \hat{\mathbf{k}} \end{pmatrix}. \tag{3.316}$$

This can be rewritten in terms of η^{μ} and the momentum vector k^{μ} as follows

$$\bar{k}^{\mu} \equiv \frac{k^{\mu} - (k\eta)\eta^{\mu}}{\sqrt{(k\eta)^2 - k^2}}\,. \tag{3.317}$$

The fixed vector eliminates the zeroth component of k^{μ}, no matter whether it is on shell or off shell.

We readily show that the polarization sum (3.314) can be rewritten as

$$\begin{aligned} P^{\mu\nu}_{\rm phys}(k) &\equiv -g^{\mu\nu} + \eta^{\mu}\eta^{\nu} - \bar{k}^{\mu}\bar{k}^{\nu} \\ &= -g^{\mu\nu} - \frac{k^{\mu}k^{\nu}}{(k\eta)^2 - k^2} + k\eta\frac{k^{\mu}\eta^{\nu} + k^{\nu}\eta^{\mu}}{(k\eta)^2 - k^2} - k^2\frac{\eta^{\mu}\eta^{\nu}}{(k\eta)^2 - k^2}, \end{aligned} \tag{3.318}$$

where the zeroth component k^0 can have any value.

3.9 MASSIVE VECTOR FIELDS

In order to understand weak interactions and some strongly interacting particles, we must also learn to describe massive vector fields (see Section 5.5). They can be electrically neutral or with electric charges ±1.

3.9.1 Action and Field Equations

The action of a neutral massive vector field $V^{\mu}(x)$ can be obtained by writing down an action like the electromagnetic one in (3.229), and simply adding a mass term:

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \left(-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}M^2 V_{\mu}V^{\mu}\right), \tag{3.319}$$

where the field tensor is now

$$F_{\mu\nu}(x) \equiv \partial_{\mu}V_{\nu}(x) - \partial_{\nu}V_{\mu}(x). \tag{3.320}$$

Charged vector fields are described by the action

$$\mathcal{A}=\int d^4x\mathcal{L}(x)=\int d^4x\left(-\frac{1}{2}F^*_{\mu\nu}F^{\mu\nu}+M^2V^*_\mu V^\mu\right). \tag{3.321}$$

In either case, the equation of motion reads

$$\partial_\mu F^{\mu\nu}+M^2V^\nu=0, \tag{3.322}$$

or more explicitly

$$[(-\partial^2-M^2)g_{\mu\nu}+\partial_\mu\partial_\nu]V^\mu(x)=0. \tag{3.323}$$

As for electromagnetic fields, the Euler-Lagrange equation for the zeroth component $V^0(x)$ does not involve the time derivative of $V^0(x)$ and is therefore not a dynamical equation, but relates $V^0(x)$ to the spatial components $V^i(x)$ and their time derivatives via

$$V^0(x)=-\partial_\mu F^{\mu 0}/M^2=\frac{1}{M^2}\left[\boldsymbol{\nabla}\cdot\dot{\mathbf{V}}(x)+\boldsymbol{\nabla}^2V^0(x)\right]. \tag{3.324}$$

In the limit $M\rightarrow 0$, this gives rise to Coulomb's law (3.257). Taking the four-divergence of (3.322), we see that the vector field $V^\mu(x)$ has no four-divergence scalar content:

$$\partial_\mu V^\mu(x)=0. \tag{3.325}$$

Physically, this eleiminates any scalar content $\partial^\mu s(x)$ from the vector potential. In contrast to the electromagnetic vector field $A^\mu(x)$, the zero four-divergence is not a matter of choice as in the Lorentz condition (3.242), but follows here from the Euler-Lagrange equations. Inserting (3.325) back into (3.323), we find that the four components of $V^\mu(x)$ satisfy the Klein-Gordon equation

$$(-\partial^2-M^2)V^\mu(x)=0, \tag{3.326}$$

which is the massive vesion of the electromagnetic field equations (3.243) in the Lorentz gauge.

3.9.2 Plane Wave Solutions for Massive Vector Fields

The plane-wave solutions look the same as in Eqs. (3.287) and (3.288) for the electromagnetic vector potential. The mass of the vector field modifies only the possible polarization vectors $\epsilon^\mu(\mathbf{k},\lambda)$. As in the electromagnetic case, the zero divergence property (3.325) eliminates one degree of freedom in the polarization vectors. It is, however, impossible to eliminate more, since there exists no gauge invariance, and thus no analog of the restricted gauge transformations (3.245). Adding to $V^\mu(x)$ a gradient $\partial^\mu\Lambda(x)$ and inserting the new field into the field equation (3.322) produces the condition $M^2\partial_\mu\Lambda(x)=0$ admitting only a trivial constant for $\Lambda(x)$. The polarization vector has therefore three independent components. Physically this reflects the fact that a massive vector particle can be studied in its rest frame. There the third component of angular momentum L_3, and the square $\mathbf{L}^2$ have three eigenstates corresponding to three linear combinations of the spatial vector components.

With the restriction (3.325) the polarization vectors satisfy $k_\mu \epsilon^\mu(\mathbf{k}, s_3) = 0$, which leaves at rest the three polarization vectors

$$\epsilon^\mu(\mathbf{0}, \pm 1) = \mp \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix}, \quad \epsilon^\mu(\mathbf{0}, 0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{3.327}$$

These are obviously eigenstates of the 4×4 angular momentum matrices L_3 and $\mathbf{L}^2$ in the defining representation (3.50)–(3.52). The relative phases have been chosen as in (3.298) to comply with the Condon-Shortley convention (see Footnote 22 and Fig. 3.3) specified in Eqs. (3.300) and (3.301) that applying L_+ to $\epsilon^\mu(\mathbf{0}, \lambda)$ leads to the states with $\lambda' = \lambda \pm 1$ with positive matrix elements $\sqrt{2}$.

The polarization vectors of momentum $\mathbf{k}$ are obtained from those at rest by applying the boost matrices (3.23):

$$\epsilon^\mu(\mathbf{k}, s_3) = B_{\hat{\mathbf{k}}}(k) \epsilon^\mu(\mathbf{0}, s_3). \tag{3.328}$$

The zero-helicity polarization vector $\epsilon^\mu(\mathbf{k}, 0)$ is also called *longitudinal polarization vector*, which is allowed for massive vector particles.

The three boosted polarization vectors satisfy the orthogonality relations

$$\epsilon_\mu(\mathbf{k}, s_3)^* \epsilon^\mu(\mathbf{k}, s_3') \;=\; -\delta_{s_3 s_3'}. \tag{3.329}$$

In order to find the completeness relations, we boost the polarization vectors at rest (3.327) to a final momentum $k^\mu \equiv (\omega_\mathbf{k}, 0, 0, k^3)$ in the z-direction using the matrix (3.14) and obtain

$$\epsilon_H^\mu(k^3 \hat{\mathbf{z}}, \pm 1) = \mp \begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix}, \qquad \epsilon_H^\mu(k^3 \hat{\mathbf{z}}, 0) = \frac{1}{M} \begin{pmatrix} k^3 \\ 0 \\ 0 \\ \omega_\mathbf{k} \end{pmatrix}, \tag{3.330}$$

where $\hat{\mathbf{z}}$ is the unit vector in the z-direction.

We can now calculate the completeness sum

$$\sum_{s_3} \epsilon^\mu(k^3 \hat{\mathbf{z}}, s_3) \epsilon^\nu(k^3 \hat{\mathbf{z}}, s_3)^* \;=\; \frac{1}{M^2} \begin{pmatrix} k^{32} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \omega_\mathbf{k}^2 \end{pmatrix}. \tag{3.331}$$

By rewriting the right-hand side in the form

$$-g^{\mu\nu} + \frac{1}{M^2} \begin{pmatrix} k^0 k^0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & k^3 k^3 \end{pmatrix} \tag{3.332}$$

we recognize the general covariant form for any direction of the momentum $\mathbf{k}$

$$\sum_{s_3}\epsilon^{\mu}(\mathbf{k},s_3)\epsilon^{\nu}(\mathbf{k},s_3)^* \;=\; P^{\mu\nu}(k)\equiv-\left(g^{\mu\nu}-\frac{k^{\mu}k^{\nu}}{M^2}\right). \tag{3.333}$$

If the vectors are first boosted into the z-direction and then rotated into the direction of their momentum

$$\hat{\mathbf{k}} \;=\; (\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta), \tag{3.334}$$

with the polar angles θ,ϕ, we obtain the polarization vectors in the helicity basis. The subsequent rotation into the direction by the trivial four-dimensional extension of the matrix (3.305) leads to the polarization vectors of helicities $\lambda=\pm1$ and 0:

$$\epsilon^{\mu}_{H}(\mathbf{k},\pm1)=\begin{pmatrix}0\\ \boldsymbol{\epsilon}(\mathbf{k},\pm1)\end{pmatrix},\qquad \epsilon^{\mu}_{H}(\mathbf{k},0)=\frac{1}{M}\begin{pmatrix}|\mathbf{k}|\\ \omega_{\mathbf{k}}\hat{\mathbf{k}}\end{pmatrix}, \tag{3.335}$$

where $\boldsymbol{\epsilon}(\mathbf{k},\pm1)$ in the transverse four-vectors with helicities $\lambda=\pm1$ are the three-dimensional polarization vectors (3.308). The polarization four-vectors $\epsilon^{\mu}_{H}(\mathbf{k},\pm1)$ agree with (3.308), the vector $\epsilon^{\mu}_{H}(\mathbf{k},0)$ is an additional *longitudinal polarization vector*.

The covariant completeness sum (3.333) can, of course, be derived directly from the general polarization vectors (3.335), whose completeness sum gives

$$\sum_{s_3}\epsilon^{\mu}(\hat{\mathbf{k}},s_3)\epsilon^{\nu}(\hat{\mathbf{k}},s_3)^* \;=\; \left(\begin{array}{c|c}|\mathbf{k}|^2/M^2 & k^0k^i\\ \hline k^ik^0/M^2 & \delta^{ij}+k^ik^j/M^2\end{array}\right), \tag{3.336}$$

which agrees with (5.579) and is the obvious rotated form of (3.332).

Let us verify that the polarization vectors $\epsilon^{\mu}(\mathbf{k},s_3)$ and its complex-conjugate $\epsilon^{\mu *}(\mathbf{k},s_3)$ lead to the correct Wigner rotations for the annihilation and creation operators $a_{\mathbf{k},s_3}$ and $b^{\dagger}_{\mathbf{k},s_3}$. These have to be the spin-1 generalizations of (3.675) and (3.681), or (3.676) and (3.677). The simplest check are the analogs of Eqs. (3.682). For this we form the 4×3 -matrices corresponding to $u(\mathbf{0})$ and $v(\mathbf{0})$ in (3.682) [recall (3.608) and (3.609)]

$$\epsilon^{\mu}(\mathbf{k})\equiv\mp\begin{pmatrix}0&0&0\\1&0&1\\i&0&-i\\0&0&0\end{pmatrix},\qquad \epsilon^{\mu *}(\mathbf{k})\equiv\mp\begin{pmatrix}0&0&0\\1&0&1\\-i&0&i\\0&0&0\end{pmatrix}. \tag{3.337}$$

Multiplying these by the 4×4 -generators [recall of (3.50)–(3.52)]

$$L_3=-i\begin{pmatrix}0&0&0&0\\0&0&1&0\\0&-1&0&0\\0&0&0&0\end{pmatrix},\; L_1=-i\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&1\\0&0&-1&0\end{pmatrix},\; L_2=-i\begin{pmatrix}0&0&0&0\\0&0&0&-1\\0&0&0&0\\0&1&0&0\end{pmatrix}. \tag{3.338}$$

from the left, we find the same result as by applying the 3 × 3 spin-1 representation matrices [recall (3.783)–(3.784)]:

$$D^j(L_3)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\ D^j(L_1)=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix},\ D^j(L_2)=\frac{-i}{\sqrt{2}}\begin{pmatrix}0&1&0\\-1&0&1\\0&-1&0\end{pmatrix}\tag{3.339}$$

from the right.

For finite Lorentz transformation, the polarization vectors undergo the Wigner rotations

$$\epsilon^\mu(\mathbf{k},s_3)\xrightarrow{\Lambda}\epsilon'^\mu(\mathbf{k},s_3)={\Lambda^\mu}_\nu\epsilon^\nu(\mathbf{k},s_3)=\sum_{s_3'=-1}^{1}\epsilon^\mu(\mathbf{p},s_3')W^{(1)}_{s_3',s_3}(p',\Lambda,p),\tag{3.340}$$

$$\epsilon^{\mu*}(\mathbf{k},s_3)\xrightarrow{\Lambda}\epsilon'^{\mu*}(\mathbf{k},s_3)={\Lambda^\mu}_\nu\epsilon^{\nu*}(\mathbf{k},s_3)=\sum_{s_3'=-1}^{1}\epsilon^{\mu*}(\mathbf{p},s_3')W^{(1)*}_{s_3',s_3}(p',\Lambda,p).\tag{3.341}$$

where $W^{(1)}_{s_3',s_3}$ is the spin-1 representation of the 2 × 2 Wigner rotations (3.675). The second transformation law follows from the first as a consequence of the reality of the Lorentz transformations ${\Lambda^\mu}_\nu$.

In closer analogy with (3.617), we can obtain the charge-conjugate polarization vectors by forming

$$\epsilon^\mu_c(\mathbf{k},s_3)\equiv-\epsilon^\mu(\mathbf{k},s_3')c^{(1)}_{s_3's_3},\tag{3.342}$$

where $c^{(s)}_{s_3's_3}$ denotes the spin-s representation of the rotation matrix $c=e^{-i\pi\sigma_2/2}$ intoduced in Eq. (3.835). It is easy to verify that $\epsilon^\mu_c(\mathbf{k},s_3)$ coincides with $\epsilon^{\mu*}(\mathbf{k},s_3)$ The matrix $c^{(s)}_{s_3's_3}$ turns the spin into the opposite direction:

$$c^{(s)}_{s_3,s_3'}=\langle s,s_3|e^{-i\hat{L}_2\pi/2}|s,s_3'\rangle=d^s_{s_3,s_3'}(\pi)=(-)^{s+s_3}\delta_{s_3,-s_3'}.\tag{3.343}$$

and has the property [recall (3.836)]:

$$D^j(R)c^{(j)}=c^{(j)}D^{j*}(R),\tag{3.344}$$

which confirms that $\epsilon^\mu_c(\mathbf{k},s_3)$ transforms with the complex-conjugate of the Wigner rotation of $\epsilon^\mu(\mathbf{k},s_3)$.

In principle, there exists also a fourth vector, called the *scalar polarization vector*, which we shall denote by and denoted by

$$\epsilon^\mu_H(\mathbf{k},s)\equiv k^\mu.\tag{3.345}$$

This polarization vector which will be of use later in Subsecs. 3.10.7 and 5.4.2. It corresponds to a pure gauge degree of freedom since in x-space it has the form $\partial^\mu\Lambda$.

As such, it transforms under an extra independent and irreducible representration of the Lorentz group descibing a scalar particle degree of freedom and no longer forms part of the vector particle. It certainly does not contribute to the gauge-invariant electromagnetic action.

Observe that for a very small mass where $\omega_{\mathbf{k}} \to |\mathbf{k}|$, the longitudinal polarization vector has the limit

$$M\epsilon^{\mu}_{H}(\mathbf{k},0) \xrightarrow{M\to 0} |\mathbf{k}| \begin{pmatrix} 1 \\ \hat{\mathbf{k}} \end{pmatrix} = k^{\mu}, \tag{3.346}$$

i.e., it goes over into the unphysical scalar degree of freedom. This is why the longitudinal polarization does not contribute to the action af a massless vector particle. In this limit, the actions (3.319) and (3.321) become invariant under local gauge tranformations of the vector field $V^{\mu}(x) \to V'^{\mu}(x) = V^{\mu}(x) + \partial^{\mu}\Lambda(x)$.

3.10 GRAVITATIONAL FIELD

The gravitational field is carried by a varying metric $g_{\mu\nu}(x)$ in spacetime. Its presence manifests itself in a local dependence of the invariant distance between events

$$(ds)^2 = g_{\mu\nu}(x)dx^{\mu}dx^{\nu}. \tag{3.347}$$

The distances in such a spacetime no longer satisfy the axioms of *Minkowski geometry* since the spacetime can have a local curvature. According to the *equivalence principle* of general relativity, the motion of point particles is independent of their mass. All point particles follow the lines of shortest distance in this geometry, the so-called *geodesics*.

The generation of the gravitational field is governed by a complicated nonlinear theory and deserves a detailed treatment on its own not to be elaborated in this text. In the present context we merely state a few relevant facts about a very weak gravitational field running through empty spacetime. It may be described by a small deviation of the metric $g_{\mu\nu}(x)$ from the Minkowski metric, which in this case is denoted by $\eta_{\mu\nu}$, for better distinction. The deviation is

$$h_{\mu\nu}(x) \equiv g_{\mu\nu}(x) - \eta_{\mu\nu}. \tag{3.348}$$

3.10.1 Action and Field Equations

The action of the field $h_{\mu\nu}(x)$ is obtained from the famous *Einstein-Hilbert action* of the graviatational field by inserting (3.348) and keeping only the quadratic terms in $h_{\mu\nu}(x)$:

$$\mathcal{A} = \int d^4x\, \mathcal{L}(x) = \frac{1}{2\kappa}\int d^4x h^{\mu\nu}G_{\mu\nu}, \tag{3.349}$$

where the constant κ is given by

$$\kappa = \frac{8\pi G}{c^3}. \tag{3.350}$$

The right-hand side contains *Newton's gravitational constant*

$$G = 6.672 \times 10^{-8}\text{cm}^3 g^{-1}\text{sec}^{-2}, \tag{3.351}$$

which is defined by the force between two planets of masses M, M' and distance r being

$$F = -GMM'/r^2.$$

Instead of κ one also uses the so-called *Planck mass*

$$M_P \equiv \sqrt{\hbar c/G} = 2.1737 \times 10^{-5} g = 1.22 \times 10^{19}\text{GeV}, \tag{3.352}$$

and writes the prefactor $1/2\kappa$ as

$$\frac{1}{2\kappa} = \frac{M_P^2}{16\pi}\frac{c^2}{\hbar}. \tag{3.353}$$

The tensor $G_{\mu\nu}$ is the so-called *Einstein tensor*

$$G_{\mu\nu} = -\frac{1}{2}\left[\partial^2 h_{\mu\nu} + \partial_\mu\partial_\nu h - \partial_\mu\partial_\lambda h^\lambda{}_\nu - \partial_\nu\partial_\lambda h^\lambda{}_\mu\right] + \frac{1}{2}\eta_{\mu\nu}(\partial^2 h - \partial_\lambda\partial_\kappa h^{\lambda\kappa}), \tag{3.354}$$

where h denotes the trace $h_\lambda{}^\lambda$. In the theory of general relativity, the Einstein tensor is closely related to the so-called *Ricci tensor* $R_{\mu\nu}$ which is the contraction of the *curvature tensor* $R_{\mu\nu\lambda}{}^\kappa$: $R_{\mu\nu} \equiv R_{\kappa\mu\nu}{}^\kappa$. The relation between $G_{\mu\nu}$ and $R_{\mu\nu}$ is

$$R_{\mu\nu} = G_{\mu\nu} - \frac{1}{2}g_{\mu\nu}G_\lambda{}^\lambda, \qquad G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R_\lambda{}^\lambda. \tag{3.355}$$

The above Einstein tensor (3.354) is the linearized version of this general tensor $G_{\mu\nu}$ arising from it by the expansion (3.348). It plays a similar role in the space of metrics $g_{\mu\nu}$ as the dual field tensor $\tilde{F}_{\mu\nu}$ does in electromagnetism. First, by analogy with (3.230), it satisfies a Bianchi identity

$$\partial_\mu G^{\mu\nu} = 0 \tag{3.356}$$

for any smooth single-valued field $h_{\mu\nu}(x)$, i.e. any field $h_{\mu\nu}(x)$ which satisfies the integrability condition $(\partial_\lambda\partial_\kappa - \partial_\kappa\partial_\lambda)h_{\mu\nu}(x) = 0$. Second, it is invariant under local gauge transformations

$$h_{\mu\nu}(x) \longrightarrow h_{\mu\nu}(x) + \partial_\mu\Lambda_\nu(x) + \partial_\nu\Lambda_\mu(x). \tag{3.357}$$

These are the linearized versions of Einstein's *general coordinate transformations*. As a consequence, the symmetric tensor $h_{\mu\nu}(x)$ carries only 6 instead of 10 independent physical components.

The field equations are obtained by variation of $\mathcal{A}$ with respect $h_{\mu\nu}(x)$:

$$\frac{\delta\mathcal{A}}{\delta h^{\mu\nu}(x)} = \frac{1}{\kappa}G^{\mu\nu}(x) = 0. \tag{3.358}$$

Thus, for a free gravitational field, the Einstein tensor vanishes, and so does the Ricci tensor, due to the relation (3.355):

$$R_{\mu\nu}(x) = 0. \tag{3.359}$$

In the presence of masses the field equation (3.358) is modified by a source term $T^{\mu\nu}$, which is simply the total symmetric energy momentum tensor of the material particles.

3.10.2 Gauge Properties

The gauge invariance of the theory under local tranformations (3.357) leaves only two dynamical degrees of freedom. To remove the gauge freedom, we choose a specific gauge, the so called *Hilbert gauge*:

$$\partial_\mu h^{\mu\nu}(x) = \frac{1}{2}\partial^\nu h(x), \qquad h(x) = h_\lambda{}^\lambda(x). \tag{3.360}$$

It corresponds to the Lorentz gauge of electromagnetism [recall (5.514)].

The Hilbert gauge can always be achieved by a gauge transformation. If $h_{\mu\nu}(x)$ is not in this gauge, we simply perform the transformation (3.357) and determine $\Lambda_\mu(x)$ from the differential equation

$$-\partial^2\Lambda^\nu(x) = \partial_\mu h^{\mu\nu}(x) - \tfrac{1}{2}\partial^\nu h(x). \tag{3.361}$$

It is useful to introduce the field

$$\phi_{\mu\nu} \equiv h_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu}h. \tag{3.362}$$

It satisfies the Hilbert condition

$$\partial^\mu\phi_{\mu\nu}(x) = 0, \tag{3.363}$$

and with this, the action reads simply

$$\mathcal{A} = \frac{1}{8\kappa}\int d^4x\partial_\lambda\phi^{\mu\nu}(x)\partial^\lambda\phi_{\mu\nu}(x). \tag{3.364}$$

Under the gauge transformations (3.357), the field $\phi_{\mu\nu}(x)$ behaves as follows:

$$\phi^{\mu\nu}(x) \to \phi^{\mu\nu}(x) + \partial^\mu\Lambda^\nu(x) + \partial^\nu\Lambda^\mu(x) - \eta^{\mu\nu}\partial_\kappa\Lambda^\kappa(x). \tag{3.365}$$

The Einstein tensor (3.354) reduces to

$$G_{\mu\nu} = -\frac{1}{2}\partial^2\phi_{\mu\nu}, \tag{3.366}$$

so that the equations of motion (3.358) become massless Klein-Gordon equations for each field component [as in Eq. (3.243) for the electromagnetic case in the Lorentz gauge]:

$$-\partial^2\phi_{\mu\nu}(x) = 0, \tag{3.367}$$

which has to be solved with the constraint (3.363).

3.10.3 Lorentz Transformation Properties of Gravitational Field

Under Lorentz transformations, $h_{\mu\nu}(x)$ behaves of course like a tensor. In a straightforward generalization of the transformation law (3.267) we may immediately write

$$h'^{\mu\nu}(x) = \Lambda^{\mu}{}_{\lambda}\Lambda^{\nu}{}_{\kappa}h^{\lambda\kappa}(\Lambda^{-1}x). \tag{3.368}$$

This transformation can be generated by analogy with (3.269) as follows:

$$h^{\mu\nu}(x) \xrightarrow{\Lambda} h'^{\mu\nu}(x) = \hat{D}(\Lambda)\Lambda^{\mu}{}_{\lambda}\Lambda^{\nu}{}_{\kappa}h^{\lambda\kappa}(x) \equiv e^{-i\frac{1}{2}\omega_{\lambda\kappa}\hat{J}^{\lambda\kappa}}h^{\mu\nu}(x), \tag{3.369}$$

with the parameters $\omega_{\mu\nu}$ specified in (3.66), (3.67), and

$$\hat{J}^{\lambda\kappa} \equiv L^{\lambda\kappa} \times 1 \times \hat{1} + 1 \times L^{\lambda\kappa} \times \hat{1} + 1 \times 1 \times \hat{L}^{\lambda\kappa}, \tag{3.370}$$

this being a direct generalization of the total angular momentum operator (3.270). The commutation rules between the generators $\hat{J}^{\mu\nu}$ are of course given by (3.272) as in the case of the vector potential.

3.10.4 Other Symmetries of Gravitational Action

Just as the scalar and electromagnetic actions, the gravitational action (3.349) is invariant under extensions of the Lorentz group.

3.10.5 Translations

Under translations (3.177),

$$x'^{\mu} = x^{\mu} + a^{\mu}, \tag{3.371}$$

the gravitational field transforms like

$$h'^{\mu\nu}(x) = h^{\mu\nu}(x-a). \tag{3.372}$$

The combination of these with Lorentz transformations forms the Poincaré group (3.181),

$$x'^{\mu} = \Lambda^{\mu}{}_{\nu}x^{\nu} + a^{\mu}, \tag{3.373}$$

under which the fields transform like

$$h'^{\mu\nu}(x) = \Lambda^{\mu}{}_{\lambda}\Lambda^{\nu}{}_{\kappa}h^{\lambda\kappa}(\Lambda^{-1}(x-a)), \tag{3.374}$$

leaving the action (3.349) invariant.

As in the scalar and vector cases (3.185) and (3.279), we can of course generate all Poincaré transformations on the field with the help of differential operators:

$$h^{\mu\nu}(x) \longrightarrow h'^{\mu\nu}(x) = \hat{D}(a)\hat{D}(\Lambda)\Lambda^{\mu}{}_{\lambda}\Lambda^{\nu}{}_{\kappa}h^{\lambda\kappa}(x) \equiv e^{ia^{\mu}\hat{p}_{\mu}/\hbar}e^{-i\frac{1}{2}\omega_{\lambda\kappa}\hat{J}^{\lambda\kappa}}h^{\mu\nu}(x), \tag{3.375}$$

with the parameters $\omega_{\mu\nu}$ specified in (3.66), (3.67).

3.10.6 Space Inversion, Time Reversal, and Charge Conjugation

Since $h_{\mu\nu}(x)$ determines the invariant distances in space via (3.347) and (3.348), it transforms like $dx_\mu dx_\nu$ under space inversion and time reversal. Under charge conjugation, it is invariant.

Thus we have under space inversion

$$h^{\mu\nu}(x) \xrightarrow{P} h'^{\mu\nu}_{P}(x) = \tilde{h}^{\mu\nu}(\tilde{x}), \tag{3.376}$$

where the tilde reverses the sign of $h^{\mu\nu}(x)$ for each spatial index, whereas under time reversal:

$$h^{\mu\nu}(x) \xrightarrow{T} h'^{\mu\nu}_{T}(x) = \tilde{h}^{\mu\nu}(x_T). \tag{3.377}$$

In principle, a tensor field $t_{\mu\nu}(x)$ has two possible transformation behaviors under space inversion:

$$t^{\mu\nu}(x) \xrightarrow{P} t'^{\mu\nu}_{P}(x) = \eta_P \tilde{t}^{\mu\nu}(\tilde{x}), \tag{3.378}$$

with $\eta_P = \pm 1$ and in the case $\eta_P = -1$ the field $t^{\mu\nu}(x)$ would have been called an *pseudotensor field*. The gravitational field $h^{\mu\nu}(x)$, however, is definitely a tensor field. This follows from its metric nature and the distance definition in (3.347), (3.348).

Similarly, the phase factor of a tensor field $t^{\mu\nu}(x)$ arising from time reversal could in principle be

$$t^{\mu\nu}(x) \xrightarrow{T} t'^{\mu\nu}_{T}(x) = \eta_T \tilde{t}^{\mu\nu}(x_T), \tag{3.379}$$

with an arbitrary phase factor η_T. For an observable real field, however, only $\eta_T = \pm 1$ are admissible. The gravitational field has $\eta_T = 1$ to preserve the definition of the distance in (3.347), (3.348) under space inversion.

Under charge conjugation, the gravitational interactions are invariant, so that

$$h^{\mu\nu}(x) \xrightarrow{C} h'^{\mu\nu}_{C}(x) = h^{\mu\nu}(x). \tag{3.380}$$

In general, a tensor field $t_{\mu\nu}(x)$ could transform like

$$t^{\mu\nu}(x) \xrightarrow{C} t'^{\mu\nu}_{C}(x) = \eta_C t^{\mu\nu}(x) \tag{3.381}$$

with $\eta_C = \pm 1$.

3.10.7 Gravitational Plane Waves

As for the previous fields, we now seek for the complete set of plane-wave solutions of the field equations (3.367) with (3.363). Since gravitons obey the zero-mass Klein-Gordon equation (3.367), the plane waves in the field $\phi^{\mu\nu}(x)$ are proportional to e^{-ikx} and e^{ikx}, with k^0 lying on the light cone $k^0 = \omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2}$. These waves are accompanied by symmetric polarization tensors $\epsilon^{\mu\nu}(\mathbf{k}, \lambda)$ which in the Hilbert gauge (3.363) satisfy the condition

$$k_\mu \epsilon^{\mu\nu}(\mathbf{k}, \lambda) = 0. \tag{3.382}$$

The label λ allows for the different polarizations. In principle, there exists 10 possibilities of forming symmetric tensors $\epsilon^{\mu\nu}(\mathbf{k},\lambda)$. The gauge condition (3.382) eliminates four of them. The remaining six components can be constructed from symmetrized tensor products of the transverse polarization vectors in (3.335) and the scalar one in (3.345) which is proportional to the zero-mass limit of the zeroth component in (3.335).

Thus we form the six symmetric combinations

$$\begin{aligned}
\epsilon_H^{\mu\nu}(\mathbf{k},2) &\equiv \epsilon_H^{\mu}(\mathbf{k},1)\epsilon_H^{\nu}(\mathbf{k},1),\\
\epsilon_H^{\mu\nu}(\mathbf{k},1) &\equiv \frac{1}{\sqrt{2}}[\epsilon_H^{\mu}(\mathbf{k},1)\epsilon_H^{\nu}(\mathbf{k},0)+(\mu\leftrightarrow\nu)],\\
\epsilon_H^{\mu\nu}(\mathbf{k},0) &\equiv \frac{1}{\sqrt{6}}[\epsilon_H^{\mu}(\mathbf{k},1)\epsilon_H^{\nu}(\mathbf{k},-1)+(\mu\leftrightarrow\nu)]+\sqrt{\frac{2}{3}}\epsilon_H^{\mu}(\mathbf{k},0)\epsilon_H^{\nu}(\mathbf{k},0),\\
\epsilon_H^{\mu\nu}(\mathbf{k},-1) &\equiv \frac{1}{\sqrt{2}}[\epsilon_H^{\mu}(\mathbf{k},-1)\epsilon_H^{\nu}(\mathbf{k},s)+(\mu\leftrightarrow\nu)],\\
\epsilon_H^{\mu\nu}(\mathbf{k},-2) &\equiv \epsilon_H^{\mu}(\mathbf{k},-1)\epsilon_H^{\nu}(\mathbf{k},-1),\\
\epsilon_H^{\mu\nu}(\mathbf{k},s) &\equiv \frac{1}{\sqrt{3}}[\epsilon_H^{\mu}(\mathbf{k},1)\epsilon_H^{\nu}(\mathbf{k},-1)+(\mu\leftrightarrow\nu)]-\sqrt{\frac{1}{3}}\epsilon_H^{\mu}(\mathbf{k},s)\epsilon_H^{\nu}(\mathbf{k},0).
\end{aligned} \tag{3.383}$$

The combinations are formed with the Clebsch-Gordan coefficients [see Appendix Appendix 3C and Table 3.2] which couple two vectors symmetrically to five components of spin 2 and one component of spin zero.

$$\begin{aligned}
|2\ 2\rangle &= |1\ 1\rangle|1\ 1\rangle,\\
|2\ 1\rangle &= \frac{1}{\sqrt{2}}\Big(|1\ 1\rangle|1\ 0\rangle+|1\ 0\rangle|1\ 1\rangle\Big)\\
|2\ 0\rangle &= \frac{1}{\sqrt{6}}\Big(|1\ 1\rangle|1\ -1\rangle+|1\ -1\rangle|1\ 1\rangle\Big)+\sqrt{\frac{2}{3}}|1\ 0\rangle|1\ 0\rangle\\
|2\ -1\rangle &= \frac{1}{\sqrt{2}}\Big(|1\ -1\rangle|1\ 0\rangle+|1\ 0\rangle|1\ -1\rangle\Big)\\
|2\ -2\rangle &= |1\ -1\rangle|1\ -1\rangle,\\
|0\ 0\rangle &= \frac{1}{\sqrt{3}}\Big(|1\ 1\rangle|1\ -1\rangle+|1\ -1\rangle|1\ 1\rangle\Big)-\frac{1}{\sqrt{3}}|1\ 0\rangle|1\ 0\rangle.
\end{aligned} \tag{3.384}$$

Since the three polarization vectors satisfy $k_\mu\epsilon_H^{\mu}(\mathbf{k},\lambda)=0$, the tensors satisfy the Hilbert gauge condition (3.382). In addition, they are traceless:

$$\epsilon_{H\mu}{}^{\mu}(\mathbf{k},\lambda)=0, \tag{3.385}$$

as follows directly from the explicit forms (3.335), (3.345) from which we find that $\epsilon_H^{\mu}(\mathbf{k},-1)\epsilon_H^{\nu}(\mathbf{k},\pm1)=0$, $\epsilon_H^{\mu}(\mathbf{k},-1)\epsilon_H^{\nu}(\mathbf{k},s)=0$, $\epsilon_H^{\mu}(\mathbf{k},s)\epsilon_H^{\nu}(\mathbf{k},s)=0$. Because of gauge invariance, not all of these tensors correspond to physical degrees of freedom. Under a gauge transformation (3.365), the Fourier transform of the field $\phi^{\mu\nu}$ receives an additional term

$$k^\mu\Lambda^\nu+k^\nu\Lambda^\mu-\eta^{\mu\nu}k_\kappa\Lambda^\kappa, \tag{3.386}$$

which cannot contribute to any observable quantities. Setting $\Lambda^\mu = \epsilon^\mu_H(\mathbf{k},1)$, $\epsilon^\mu_H(\mathbf{k},-1)$, and $\epsilon^\mu_H(\mathbf{k},s)$, and using (3.382), we see that the three combinations (3.386) become precisely the polarization tensors $\epsilon^{\mu\nu}_H(\mathbf{k},\pm1)$ and $\epsilon^{\mu\nu}_H(\mathbf{k},s)$, respectively.

But also the polarization tensor $\epsilon^\mu_H(\mathbf{k},0)$ is unphysical. This is seen by introducing a forth linearly independent polarization "vector"

$$\epsilon^\mu_H(\mathbf{k},\bar{s}) = (k^0,-\mathbf{k}). \tag{3.387}$$

The name "vector" is set in quotation marks since it indicates here merely a four-component object. It does not mean that $\epsilon^\mu_H(\mathbf{k},\bar{s})$ behaves like a vector under Lorentz transformations. This can be seen most easily by forming the product

$$\epsilon_{H\mu}(\mathbf{k},s)\epsilon^\mu_H(\mathbf{k},\bar{s}) = k^{02} + \mathbf{k}^2 = 2\mathbf{k}^2,$$

which is not Lorentz-invariant. We shall call the "vector" $\epsilon^\mu_H(\mathbf{k},\bar{s})$ an antiscalar polarization vector. The four "vectors" $\epsilon^\mu_H(\mathbf{k},\pm1)$, $\epsilon^\mu_H(\mathbf{k},s)$, $\epsilon^\mu_H(\mathbf{k},\bar{s})$ form a complete basis in the space of polarization vectors. This is compactly expressed in the completeness relation

$$\epsilon^\nu_H(\mathbf{k},1)\epsilon^\nu_H(\mathbf{k},-1)+\epsilon^\nu_H(\mathbf{k},-1)\epsilon^\nu_H(\mathbf{k},1)+\frac{1}{2\mathbf{k}^2}[\epsilon^\mu_H(\mathbf{k},s)\epsilon^\nu_H(\mathbf{k},\bar{s})+(\mu\leftrightarrow\nu)]=\eta^{\mu\nu}. \tag{3.388}$$

The first two terms on the left-hand side can obviously be replaced by the polarization tensor $\epsilon^{\mu\nu}_H(\mathbf{k},0)$, so that (3.388) may be rewritten as

$$\epsilon^{\mu\nu}_H(\mathbf{k},0) = \eta^{\mu\nu} - \frac{1}{2\mathbf{k}^2}[\epsilon^\mu_H(\mathbf{k},s)\epsilon^\nu_H(\mathbf{k},\bar{s}) + (\mu\leftrightarrow\nu)]. \tag{3.389}$$

Inserting on the right-hand side the explicit form $\epsilon^\mu_H(\mathbf{k},s) = k^\mu$ for the scalar polarization vector (3.345), and setting $\epsilon^\mu_H(\mathbf{k},\bar{s})/2\mathbf{k}^2 = \Lambda^\mu$, the right-hand side can be rewritten as $\eta^{\mu\nu}k_\kappa\Lambda^\kappa - k^\mu\Lambda^\nu - k^\nu\Lambda^\mu$, thus demonstrating that the polarization tensor $\epsilon^{\mu\nu}_H(\mathbf{k},0)$ is of the pure gauge form (3.386), and thus unphysical.

Thus we remain with only two physical polarization tensors $\epsilon^{\mu\nu}_H(\mathbf{k},\pm2)$. These describe gravitational waves with helicities $\lambda = \pm2$. An analysis of the temporal behavior of the fields shows that the tensors $\epsilon^{\mu\nu}_H(\mathbf{k},\pm2)$ give the gravitational waves a circular polarization, this being analogous to the circularly polarized light described by plane electromagnetic waves with polarization vectors $\epsilon^\mu_H(\mathbf{k},\pm1)$ as discussed in Section 3.8.

In electromagnetism, one often descibes plane wave with real polarization vectors

$$\epsilon^\mu_H(\mathbf{k},1) = -[\epsilon^\mu_H(\mathbf{k},+1) + \epsilon^\mu_H(\mathbf{k},-1)], \qquad \epsilon^\mu_H(\mathbf{k},2) = i[\epsilon^\mu_H(\mathbf{k},+1) - \epsilon^\mu_H(\mathbf{k},-1)], \tag{3.390}$$

corresponding to linearly polarized light waves whose field vectors oscillate along the directions orthogonal to the momentum $\mathbf{k}$. By analogy, we introduce the real combinations of the two physical polarization tensors

$$\begin{aligned}\epsilon^{\mu\nu}_{H+}(\mathbf{k}) &\equiv \frac{1}{\sqrt{2}}[\epsilon^{\mu\nu}_H(\mathbf{k},+2) + \epsilon^{\mu\nu}_H(\mathbf{k},-2)]\\ \epsilon^{\mu\nu}_{H\times}(\mathbf{k}) &= \frac{1}{\sqrt{2}i}[\epsilon^{\mu\nu}_H(\mathbf{k},2) - \epsilon^{\mu\nu}_H(\mathbf{k},-2)].\end{aligned} \tag{3.391}$$

An analysis of the motion of a circular ring of mass points in a plane gravitational field $g_{\mu\nu}(x) = \eta_{\mu\nu} + h_{\mu\nu}(x)$ with the polarization tensors (3.391) reveils that $\epsilon^{\mu\nu}_{H+}(\mathbf{k})\epsilon^{\mu\nu}_{H\times}(\mathbf{k})$ corresponds to waves distorting the circular ring periodically into an ellipsoidal one, with vertical and horizontal axes, whereas $\epsilon^{\mu\nu}_{H\times}(\mathbf{k})$ does the same with the axes rotated by 45 degrees.

In a circularly polarized wave with polarization tensors $\epsilon^{\mu\nu}_{H}(\mathbf{k}, \pm 2)$ rotates anticlockwise or clockwise around the momentum direction, depending on the helicity of the incoming wave.

3.11 RELATIVISTIC FREE FERMI FIELDS

For Fermi fields, the situation is technically more involved. Experimentally, fermions always have an even number of spin degrees of freedom. We shall denote the associated field by ψ_a, where the index a labels the different spin components. Under rotations, these spin components are transformed into each other, as observed experimentally in the *Stern-Gerlach experiment*. We shall see below that Lorentz transformations also lead to certain well-defined mixtures of different spin components.

The question arises whether we can construct a Lorentz-invariant action involving $(2s+1)$ spinor field components. To see the basic construction principle we use the known transformation law (3.267) for the four-vector field A^μ as a guide. For an arbitrary *spinor field* we postulate the transformation law

$$\psi_a(x) \xrightarrow{\Lambda} \psi'_a(x') = D_{ab}(\Lambda)\psi_b(x), \tag{3.392}$$

with an appropriate $(2s+1) \times (2s+1)$ spinor transformation matrix $D_{ab}(\Lambda)$ which we have to construct. This can be done by using purely mathematical arguments. The construction is the subject of the so-called *group representation theory*. First of all, we perform two successive Lorentz transformations,

$$x'' = \Lambda x = \Lambda_2 x' = \Lambda_2 \Lambda_1 x. \tag{3.393}$$

Since the Lorentz transformations Λ_1, Λ_2 are elements of a group, the product $\Lambda \equiv \Lambda_2\Lambda_1$ is again a Lorentz transformation. Under the individual factors Λ_2 and Λ_1, the field transforms as

$$\begin{aligned} \psi(x) \xrightarrow{\Lambda_1} \psi'(x') &= D(\Lambda_1)\psi(x), \\ \psi'(x') \xrightarrow{\Lambda_2} \psi''(x'') &= D(\Lambda_2)\psi'(x'), \end{aligned} \tag{3.394}$$

so that under $\Lambda = \Lambda_2\Lambda_1$,

$$\psi(x) \xrightarrow{\Lambda_2\Lambda_1} \psi''(x'') = D(\Lambda_2)D(\Lambda_1)\psi(x). \tag{3.395}$$

For the combined Λ, the transformation matrix is $D(\Lambda)$, bringing the field to

$$\psi''(x'') = D(\Lambda_2\Lambda_1)\psi(x). \tag{3.396}$$

Comparing this with (3.395) shows that the matrices $D(\Lambda)$ which mix the spinor field components under the Lorentz group must follow a group multiplication law which has to be compatible with that of the group itself. The mapping

$$\Lambda \longrightarrow D(\Lambda) \tag{3.397}$$

is a homomorphism, and the $D(\Lambda)$'s form a *matrix representation* of the group.

Note that the transformation law (3.267) for the vector field $A^\mu(x)$ follows the same rule with

$$D(\Lambda) \equiv \Lambda = e^{-i\frac{1}{2}\omega_{\mu\nu}L^{\mu\nu}} \tag{3.398}$$

being the defining 4 × 4 -representation of the Lorentz group. The parameters $\omega_{\mu\nu}$ are specified in (3.66), (3.67).

The scalar field transformation law (3.46) follows trivially the same rule, where $D(\Lambda) \equiv 1$ is the identity representation.

The group laws for Λ and $D(\Lambda)$ are sufficiently stringent to allow only for a countable set of *fundamental*[9] finite-dimensional transformation matrices $D(\Lambda)$. Below we shall see that these are characterized by two quantum numbers, s_1 and s_2, either one of these taking all possible half-integer or integer values $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. The representation spaces associated with $D^{(s_1,s_2)}(\Lambda)$ will turn out to harbor particles of spins $|s_1 - s_2|$ to $s_1 + s_2$. Hence, particles with a single fixed spin s can only follow the $D^{(s,0)}(\Lambda)$ or $D^{(0,s)}(\Lambda)$ transformation laws.

From the development in Sections 3.18 and 3.19 we know how the representation matrices $D^{(s_1,s_2)}(\Lambda)$ are most efficiently constructed. We have to determine all possible sets of six matrices which satisfy the commutation relations (3.82). Any set of such matrices forms a representation of the Lie algebra defined by (3.82).

In this general framework, the scalar particles studied so far transform with the trivial representation $D^{(0,0)}(\Lambda) \equiv 1$ of the Lorentz group. They are said to have spin zero.

Let us now study the smallest nontrivial representation.

3.12 SPIN-1/2 FIELDS

The smallest matrices satisfying the subalgebra (3.72) associated with the rotation subgroup of the Lorentz group are

$$L_i = \frac{\sigma^i}{2}, \tag{3.399}$$

where σ^i are the *Pauli matrices*

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.400}$$

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[9] Mathematically, *fundamental* means that the representation is irreducible. Any arbitrary representation is equivalent to a direct sum of irreducible ones.

The two-component basis on which $\mathbf{L}^2$ and L_3 are diagonal, with eigenvalues 3/4 and ±1/2, respectively, are the Pauli spinors

$$\chi(\tfrac{1}{2}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi(-\tfrac{1}{2}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.401}$$

The full Lie algebra (3.72)–(3.74) can be satisfied in two inequivalent ways. Either

$$M_i = -i\sigma^i/2, \tag{3.402}$$

or

$$M_i = i\sigma^i/2. \tag{3.403}$$

The first representation

$$(L_i, M_i) = \left(\frac{\sigma^i}{2}, -i\frac{\sigma^i}{2}\right) \tag{3.404}$$

is denoted by $(\frac{1}{2}, 0)$, the second one

$$(L_i, M_i) = \left(\frac{\sigma^i}{2}, i\frac{\sigma^i}{2}\right) \tag{3.405}$$

by $(0, \frac{1}{2})$. Exponentiating these generators we obtain the global representations of the Lorentz group

$$D^{(\frac{1}{2},0)}(\Lambda) = e^{-i(\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2 - i\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2)}, \tag{3.406}$$

$$D^{(0,\frac{1}{2})}(\Lambda) = e^{-i(\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2 + i\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2)}. \tag{3.407}$$

An alternatively decomposition which will later be useful is a factorization into rotations and subsequent boost:

$$D^{(\frac{1}{2},0)}(\Lambda) = e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2} e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2}, \tag{3.408}$$

$$D^{(0,\frac{1}{2})}(\Lambda) = e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2} e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2}. \tag{3.409}$$

The right-hand sides can easily be calculated explicitly by expanding them in a Taylor series. The expansion terms separate naturally into even and odd powers due to the normalization property of the $\boldsymbol{\sigma}$-matrices $(\hat{\boldsymbol{\varphi}}\boldsymbol{\sigma})^2 = 1$, $(\hat{\boldsymbol{\zeta}}\boldsymbol{\sigma})^2 = 1$, where $\hat{\boldsymbol{\varphi}}$, $\hat{\boldsymbol{\zeta}}$ are the directions of rotation axis and Lorentz boost, respectively. For rotations, this implies that for integer k: $(\boldsymbol{\varphi}\boldsymbol{\sigma})^{2k} = \varphi^{2k}$, $(\boldsymbol{\varphi}\boldsymbol{\sigma})^{2k+1} = (\hat{\boldsymbol{\varphi}}\boldsymbol{\sigma})\,\varphi^{2k+1}$, so that

$$e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \left(\frac{\hat{\boldsymbol{\varphi}}\boldsymbol{\sigma}}{2}\right)^n = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \left(\frac{\varphi}{2}\right)^{2k} - i\hat{\boldsymbol{\varphi}}\boldsymbol{\sigma} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \left(\frac{\varphi}{2}\right)^{2k+1}. \tag{3.410}$$

Summing up even and odd powers of the parameters φ separately, this becomes

$$R_{\hat{\boldsymbol{\varphi}}}(\varphi) = e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2} \;=\; \cos\frac{\varphi}{2} - i\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\varphi}}\sin\frac{\varphi}{2}. \tag{3.411}$$

Similarly:

$$B_{\hat{\zeta}}(\zeta) = e^{\mp\zeta\cdot\boldsymbol{\sigma}/2} \;=\; \cosh\frac{\zeta}{2} \mp \boldsymbol{\sigma}\cdot\hat{\boldsymbol{\zeta}}\sinh\frac{\zeta}{2}. \tag{3.412}$$

When applying these representations to a particle of mass M at rest, energy and momentum are boosted from $p^\mu = (M, \mathbf{0})$ to

$$p^\mu = (p^0, \mathbf{p}) = M(\cosh\zeta, \hat{\boldsymbol{\zeta}}\sinh\zeta). \tag{3.413}$$

Using the relations

$$\begin{aligned}\cosh\frac{\zeta}{2} &= \sqrt{\frac{1}{2}(\cosh\zeta + 1)} = \sqrt{\frac{p_0 + M}{2M}},\\ \sinh\frac{\zeta}{2} &= \sqrt{\frac{1}{2}(\cosh\zeta - 1)} = \sqrt{\frac{p_0 - M}{2M}},\end{aligned} \tag{3.414}$$

we can express the pure Lorentz transformations of the $(\frac{1}{2}, 0)$-representation in terms of energy and momentum of the boosted particle as follows:

$$B_{\hat{\zeta}}(\zeta) = e^{-\zeta\cdot\boldsymbol{\sigma}/2} = \frac{1}{\sqrt{2M(p_0 + M)}}(p_0 + M - \boldsymbol{\sigma}\cdot\mathbf{p}). \tag{3.415}$$

We may also use the Einstein parameter γ to write this as

$$B_{\hat{\zeta}}(\zeta) == \frac{1}{\sqrt{2(\gamma+1)}}(\gamma + 1 - \gamma\boldsymbol{\sigma}\cdot\mathbf{v}/c). \tag{3.416}$$

It is convenient to introduce an extra 2 × 2 "Pauli matrix"

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.417}$$

and define a *four-vector of matrices*

$$\sigma^\mu \equiv (\sigma^0, \sigma^i). \tag{3.418}$$

With these, we can form *Lorentz-invariant matrices*

$$p\sigma \equiv p_\mu\sigma^\mu = p^\mu\sigma_\mu. \tag{3.419}$$

This notation allows us to write the boosts in the $(\frac{1}{2}, 0)$-representation of the Lorentz group as

$$e^{-\zeta\cdot\boldsymbol{\sigma}/2} = \frac{M + p\sigma}{\sqrt{2M(p_0 + M)}}, \tag{3.420}$$

For a corresponding expression in the $(0,\frac{1}{2})$-representation we define, by analogy with $\tilde{x} \equiv (x^0, -x^i)$ in Eq. (3.187), the space inverted vectors:

$$\begin{aligned} \tilde{p}^\mu &\equiv (p^0, -p^i), \\ \tilde{\sigma}^\mu &= (\sigma^0, -\sigma^i). \end{aligned} \tag{3.421}$$

Then:

$$e^{\zeta\cdot\boldsymbol{\sigma}/2} = \frac{M + \tilde{p}\sigma}{\sqrt{2M(p_0+M)}} = \frac{M + p\tilde{\sigma}}{\sqrt{2M(p_0+M)}}. \tag{3.422}$$

For many explicit calculations to follow it is useful to realize that the boost matrices (3.420) and (3.422) may be considered as the square root of the same expression with twice the rapidity

$$e^{\mp\zeta\cdot\boldsymbol{\sigma}} = \cosh\zeta \mp \boldsymbol{\sigma}\cdot\hat{\boldsymbol{\zeta}}\sinh\zeta. \tag{3.423}$$

Because of (3.413), the right-hand sides have simple momentum representations

$$e^{-\zeta\cdot\boldsymbol{\sigma}} = \frac{p\sigma}{M}, \qquad e^{\zeta\cdot\boldsymbol{\sigma}} = \frac{p\tilde{\sigma}}{M}. \tag{3.424}$$

Using these we may write the boost matrices shorter as

$$e^{-\zeta\cdot\boldsymbol{\sigma}/2} = \sqrt{\frac{p\sigma}{M}}, \qquad e^{\zeta\cdot\boldsymbol{\sigma}/2} = \sqrt{\frac{p\tilde{\sigma}}{M}}, \tag{3.425}$$

a notation which will be convenient in later calculations.

Having thus succeeded in finding the smallest dimensional representations of the Lorentz group, we define fields $\xi_\alpha(x)$ and $\eta^{\dot{\alpha}}(x)$ to have the corresponding transformation laws

$$\begin{aligned} \xi_\alpha(x) &\xrightarrow{\Lambda} \xi'_\alpha(x') = D^{(\frac{1}{2},0)}(\Lambda)_\alpha{}^\beta\,\xi_\beta(x), \\ \eta^{\dot{\alpha}}(x) &\xrightarrow{\Lambda} \eta'^{\dot{\alpha}}(x') = D^{(0,\frac{1}{2})}(\Lambda)^{\dot{\alpha}}{}_{\dot{\beta}}\,\eta^{\dot{\beta}}(x). \end{aligned} \tag{3.426}$$

The different transformation behavior of the two kinds of spinors is exhibited by the lower undotted and upper dotted indices. These spinors were introduced by Weyl,[10] and are referred to as *Weyl spinors* of type $(\frac{1}{2},0)$ and $(0,\frac{1}{2})$, respectively.

Let us now see whether we can construct a Lorentz-invariant free-field action from Weyl spinors which can contain only quadratic terms in the fields and their first derivatives. First we look for invariant quadratic terms without spacetime derivatives, which are needed to describe particles with a mass. Let us begin by looking for suitable combinations of ξ and η. which are invariant only under the rotation subgroup. For this, the representation matrices $D^{(\frac{1}{2},0)}$ and $D^{(0,\frac{1}{2})}$ are both equal to the same unitary matrix $U = e^{-i\zeta\cdot\boldsymbol{\sigma}/2}$ to be applied to both ξ and η. Due to the unitarity of U, all quadratic expressions $\xi^\dagger\xi$, $\eta^\dagger\eta$, $\eta^\dagger\xi$, $\xi^\dagger\eta$ are rotationally invariant quadratic field combinations, for example,

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[10] H. Weyl, J. Phys. *50*, 330 (1929).

$$\begin{aligned} \xi'^\dagger(x')\xi'(x') &= \xi^\dagger(x)U^\dagger U\xi(x) \\ &= \xi^\dagger(x)\xi(x). \end{aligned} \tag{3.427}$$

Consider now pure Lorentz transformations. Then $D^{(\frac{1}{2},0)} = e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}$ and $D^{(0,\frac{1}{2})} = e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}$ are both nonunitary but hermitian. The quadratic expressions $\xi^\dagger\xi$ and $\eta^\dagger\eta$ are no longer invariant. However, since the two representation matrices are inverse to each other,

$$D^{(\frac{1}{2},0)\dagger} = D^{(\frac{1}{2},0)} = D^{(0,\frac{1}{2})^{-1}}, \tag{3.428}$$

the mixed quadratic expressions $\eta^\dagger\xi$ and $\xi^\dagger\eta$ are invariant field combinations. Thus we conclude: If the action is to contain a quadratic field combination without spacetime derivatives then both spinors ξ, η, i.e. four field components $\xi_1, \xi_2, \eta^1, \eta^2$, are necessary to form an invariant.

Let us now construct a Lorentz invariant term involving spacetime derivatives ∂_μ. It is necessary if an action is to describe a particle which can move through spacetime. Consider first the spatial derivatives. It is easy to see that

$$\begin{aligned} &\xi^\dagger\sigma^i\partial_i\xi, \quad \eta^\dagger\sigma^i\partial_i\eta, \\ &\xi^\dagger\sigma^i\partial_i\eta, \quad \eta^\dagger\sigma^i\partial_i\xi, \end{aligned} \tag{3.429}$$

are all rotationally invariant. Take for example

$$\xi^{\dagger\prime}(x')\sigma^i\partial_i'\xi'(x') = \xi^\dagger(x)U^\dagger\sigma^i\partial_i'U\xi(x). \tag{3.430}$$

From the commutation rules among the Pauli matrices σ^i it is easy to derive the transformation law

$$U^{-1}\sigma^i U = R_{\hat{\boldsymbol{\varphi}}}(\varphi)^i{}_j\sigma^j. \tag{3.431}$$

The proof of this proceeds in the same way as in the finite transformation of the spatial vector x^i in (3.100) with the help of Lie's expansion formula (3.99). The commutation rules between $-i\sigma^3/2$ and σ^i are precisely the same as those between $\hat{L}_3$ and x^i, so that we find for a rotation around the 3-axis,

$$\begin{aligned} e^{i\sigma^3\varphi/2}\sigma^3 e^{-i\sigma^3\varphi/2} &= \sigma^3, \\ e^{i\sigma^3\varphi/2}\sigma^1 e^{-i\sigma^3/2\varphi} &= \cos\varphi\,\sigma^1 - \sin\varphi\,\sigma^2, \\ e^{i\sigma^3\varphi/2}\sigma^2 e^{-i\sigma^3\varphi/2} &= \sin\varphi\,\sigma^1 + \cos\varphi\,\sigma^2, \end{aligned} \tag{3.432}$$

corresponding precisely to (3.431) with the matrix (3.8). The 2×2 representation has the advantage used already in (3.411) that the exponentials can be expanded into linear combinations of σ^0 and σ^i. If we do this on the left-hand sides, we can calculate the right-hand sides also using products of σ^i rather than commutators as in Lie's expansion formula (3.99).

Now, since derivatives transform like a vector,

$$\partial_i \xrightarrow{R} \partial_i' = R_{\hat{\varphi}}(\varphi)_{ij}\partial_j, \tag{3.433}$$

the expression (3.430) is indeed a rotationally invariant field combination. For the other terms in (3.429), the proof is the same.

How can we extend the expressions (3.429) to form relativistic invariants? For this we remember that in the boost matrices (3.425), the four-vector generalizations $\sigma^\mu, \tilde{\sigma}^\mu$ of the Pauli matrices appeared naturally contracted with p_μ. This suggests studying

$$\begin{array}{ll} \xi^\dagger\sigma^\mu\partial_\mu\xi, & \eta^\dagger\sigma^\mu\partial_\mu\eta, \\ \xi^\dagger\sigma^\mu\partial_\mu\eta, & \eta^\dagger\sigma^\mu\partial_\mu\xi, \end{array} \tag{3.434}$$

and once more the same combinations but with σ^μ replaced by $\tilde{\sigma}^\mu$.
The additional time derivatives in (3.434) are trivially invariant under rotations and thus do not destroy the rotational invariance of the spatial parts shown in (3.430). Consequently we have to study only the behavior under pure Lorentz transformations in, say, the z-direction. Under these, the x- and y-components do not change. It is easy to verify that

$$\begin{aligned} e^{-\sigma^3\zeta/2}\sigma^0 e^{-\sigma^3\zeta/2} &= e^{-\sigma^3\zeta} = \cosh\zeta\,\sigma^0 + \sinh\zeta\,(-\sigma^3), \\ e^{-\sigma^3\zeta/2}(-\sigma^3)e^{-\sigma^3\zeta/2} &= e^{-\sigma^3\zeta}(-\sigma^3) = \sinh\zeta\,\sigma^0 + \cosh\zeta\,(-\sigma^3), \\ e^{\sigma^3\zeta/2}\sigma^0 e^{\sigma^3\zeta/2} &= e^{\sigma^3\zeta} = \cosh\zeta\,\sigma^0 + \sinh\zeta\,\sigma^3, \\ e^{\sigma^3\zeta/2}\sigma^3 e^{\sigma^3\zeta/2} &= e^{\sigma^3\zeta}\sigma^3 = \sinh\zeta\,\sigma^0 + \cosh\zeta\,\sigma^3. \end{aligned} \tag{3.435}$$

In contrast to the transformation laws (3.432), this cannot be derived with the help of Lie's expansion formula (3.99), since the exponentials on the left-hand sides have the same exponents. However, as before in the calculation of (3.412), we may use the multiplicative algebra of σ^i-matrices rather than the commutation rules between them to expand the exponentials to expand the exponentials into linear combinations of σ^0 and σ^i. and calculate (3.435).

The first two lines in (3.435) show that the matrices $\tilde{\sigma}^\mu$ transform like a four-vector under $(\frac{1}{2},0)$-boosts, the remaining lines that σ^μ do the same under $(0,\frac{1}{2})$-boosts. In combination with rotations, we thus have proved the Lorentz transformation behavior:

$$\begin{aligned} D^{(\frac{1}{2},0)\dagger}(\Lambda)\tilde{\sigma}^\mu D^{(\frac{1}{2},0)}(\Lambda) &= \Lambda^\mu{}_\nu\tilde{\sigma}^\nu, \\ D^{(0,\frac{1}{2})\dagger}(\Lambda)\sigma^\mu D^{(0,\frac{1}{2})}(\Lambda) &= \Lambda^\mu{}_\nu\sigma^\nu, \end{aligned} \tag{3.436}$$

This allows us to conclude that the quadratic field terms with a derivative

$$\xi^\dagger\tilde{\sigma}^\mu\partial_\mu\xi, \quad \eta^\dagger\sigma^\mu\partial_\mu\eta \tag{3.437}$$

are Lorentz-invariant. For instance

$$\begin{aligned}\eta'^{\dagger}(x')\sigma^{\mu}\partial'_{\mu}\eta'(x') &= \eta^{\dagger}(x)D^{(0,\frac{1}{2})\dagger}(\Lambda)\sigma^{\mu}\partial'_{\mu}D^{(0,\frac{1}{2})}(\Lambda)\eta(x)=\eta^{\dagger}(x)\Lambda^{\mu}{}_{\nu}\sigma^{\nu}\partial'_{\mu}\eta(x)\\ &= \eta^{\dagger}(x)\sigma^{\nu}\partial_{\nu}\eta(x). \qquad (3.438)\end{aligned}$$

It is easy to see that the other quadratic combinations in (3.434) are not invariant.

If we allow only for these lowest-order in the derivative terms, the most general Lorentz-invariant action reads

$$\mathcal{A}=\int d^4x\,\mathcal{L}(x)=\int d^4x\,(\xi^{\dagger}\tilde{\sigma}^{\mu}i\partial_{\mu}\xi+\eta^{\dagger}\sigma^{\mu}i\partial_{\mu}\eta-M_1\xi^{\dagger}\eta-M_2\eta^{\dagger}\xi). \qquad (3.439)$$

Observe that this expression involves necessarily both two-component spinors ξ and η. Only for zero parameters $M_{1,2}$, a single species of two-component spinors ξ *or* η possesses an invariant action.

The equations of motion are obviously

$$\begin{aligned}i\tilde{\sigma}^{\mu}\partial_{\mu}\xi(x) &= M_1\eta(x),\\ i\sigma^{\mu}\partial_{\mu}\eta(x) &= M_2\xi(x). \qquad (3.440)\end{aligned}$$

Combining the second equation with the first and vice versa we find the two second-order field equations

$$(-\partial^2-M_1M_2)\xi(x) = 0, \qquad (3.441)$$
$$(-\partial^2-M_1M_2)\eta(x) = 0. \qquad (3.442)$$

In deriving these, we have used the relation

$$\sigma^{\mu}\tilde{\sigma}^{\nu}+\sigma^{\nu}\tilde{\sigma}^{\mu}=2g^{\mu\nu}, \qquad (3.443)$$

by which

$$\tilde{\sigma}^{\mu}\partial_{\mu}\sigma^{\nu}\partial_{\nu}=\partial^2. \qquad (3.444)$$

which is easily proved by direct evaluation. In momentum space, equations (3.441) are solved by particles of mass

$$M=\sqrt{M_1M_2}. \qquad (3.445)$$

For $M\neq 0$, it is useful to combine the two spinors ξ and η into a single four-component object, called *bispinor* or *Dirac spinor*:

$$\psi(x)=\begin{pmatrix}\xi(x)\\ \eta(x)\end{pmatrix}. \qquad (3.446)$$

In terms of this, the action may be written as

$$\mathcal{A}=\int d^4x\,\mathcal{L}(x)=\int d^4x\,\bar{\psi}(x)\left[i\gamma^{\mu}\partial_{\mu}-\begin{pmatrix}M_2 & 0\\ 0 & M_1\end{pmatrix}\right]\psi(x), \qquad (3.447)$$

where γ^μ are the 4×4 *Dirac matrices*:

$$\gamma^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \tilde{\sigma}^\mu & 0 \end{pmatrix}, \tag{3.448}$$

and $\bar{\psi}(x)$ is the *adjoint* Dirac spinor defined by

$$\bar{\psi}(x) \equiv \psi^\dagger(x)\gamma^0 = (\eta^\dagger(x), \xi^\dagger(x)). \tag{3.449}$$

The Dirac matrices satisfy the anticommutation rules

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \tag{3.450}$$

It has become customary to abbreviate the contraction of γ^μ with any vector v^μ by

$$\not{v} \equiv \gamma^\mu v_\mu. \tag{3.451}$$

In this notation, the derivative terms $\gamma^\mu \partial_\mu$ in (3.447) becomes simply $\not{\partial}$.

For the Dirac spinor, the equations of motion (3.440) take the form

$$\left[i\not{\partial} - \begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} \right] \psi(x) = 0. \tag{3.452}$$

This is almost, but not quite, the wave equation postulated first by Dirac for the electron. He assumed a diagonal 4×4 -mass matrix

$$\begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} = M \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.453}$$

and proposed the *Dirac equation*

$$(i\not{\partial} - M)\, \psi(x) = 0 \tag{3.454}$$

corresponding to an action

$$\mathcal{A} = \int d^4x\, \mathcal{L}(x) = \int d^4x\, \bar{\psi}(x)\, (i\not{\partial} - M)\, \psi(x). \tag{3.455}$$

Just as in the case of a complex scalar field, there exists a four-vector quantity

$$j^\mu(x) = \bar{\psi}(x)\gamma^\mu\psi(x), \tag{3.456}$$

which by virtue of the Dirac equation satisfies a local conservation law [recall (3.164) and (3.165)]

$$\partial_\mu j^\mu(x) = 0. \tag{3.457}$$

This four-vector will be used in 10 to couple Dirac fields to electromagnetism, thus becoming the electromagnetic current density of the Dirac field. Later in Subsec. 6.11.1 we shall see that the local conservation law (3.457) is a consequence of the invariance of the Dirac action (3.455) under arbitrary changes of the phase of the field

$$\psi(x) \rightarrow e^{-i\alpha}\psi(x). \tag{3.458}$$

It is this invariance which gives rise to a conserved current density [see (6.243), also (10.46)].

By construction, the actions (3.447) and (3.455) are invariant under the bispinor or Dirac-Lorentz transformations

$$\psi_a(x) \xrightarrow{\Lambda} \psi'_a(x') = D_a{}^b(\Lambda)\psi_b(x), \tag{3.459}$$

where the 4×4 -matrices $D(\Lambda)$ consists of rotations and pure Lorentz transformations

$$D(R) = \begin{pmatrix} e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2} & 0 \\ 0 & e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2} \end{pmatrix}, \qquad D(B) = \begin{pmatrix} e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2} & 0 \\ 0 & e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2} \end{pmatrix}. \tag{3.460}$$

With the 2 × 2 matrices (3.408) and (3.409) we can write $D(\Lambda)$ in the form

$$D(\Lambda) = \begin{pmatrix} D^{(\frac{1}{2},0)}(\Lambda) & 0 \\ 0 & D^{(0,\frac{1}{2})}(\Lambda) \end{pmatrix}, \tag{3.461}$$

The invariance can be seen most directly by combining the transformation laws (3.436) to the 4 × 4 -form

$$\bar{D}(\Lambda)\gamma^\mu D(\Lambda) = \Lambda^\mu{}_\nu \gamma^\nu. \tag{3.462}$$

where we define

$$\bar{D}(\Lambda) \equiv \begin{pmatrix} D^{(\frac{1}{2},0)\dagger}(\Lambda) & 0 \\ 0 & D^{(0,\frac{1}{2})\dagger}(\Lambda) \end{pmatrix} = D^{-1}(\Lambda). \tag{3.463}$$

From (3.462), the invariance of the derivative term in (3.455) follows at once, using (3.132), (3.133), and (3.40):

$$\begin{aligned} i\bar{\psi}'(x')\gamma^\mu\partial'_\mu\psi'(x') &= i\bar{\psi}(x)\bar{D}(\Lambda)\gamma^\mu D(\Lambda)\partial'_\mu\psi(x) = i\bar{\psi}(x)\Lambda^\mu{}_\nu\gamma^\nu\partial'_\mu\psi(x) \\ &= i\bar{\psi}(x)\gamma^\nu\partial_\nu\psi(x). \end{aligned} \tag{3.464}$$

In terms of Dirac matrices (3.448), the pure Lorentz transformations can also be written as

$$D(B) = \frac{M + \not{p}\gamma^0}{\sqrt{2M(p_0+M)}}. \tag{3.465}$$

The representation matrices of all Lorentz transformations may be expressed in terms of covariant generators as

$$D(\Lambda) = e^{-i\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}, \tag{3.466}$$

where $\omega_{\mu\nu}$ is the same antisymmetric matrix as in (3.65) containing both the rotation and boost parameters as specified in (3.66) and (3.67). Taking the matrices (3.460) to the limit of small $\boldsymbol{\varphi}$ and $\boldsymbol{\zeta}$, we identify the 4×4-matrix generators $S^{\mu\nu}$ as

$$S^{ij} = \epsilon_{ijk}\,\frac{1}{2}\begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}, \quad S^{0i} = \frac{i}{2}\begin{pmatrix} -\sigma^i & 0 \\ 0 & \sigma^i \end{pmatrix}. \tag{3.467}$$

The 4×4 -generator of the rotation group on the left-hand side contains the direct 4×4 -extension of the Pauli matrices is denoted by

$$\boldsymbol{\Sigma} \equiv \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \tag{3.468}$$

and the spin matrix

$$\mathbf{S} \equiv \frac{1}{2}\boldsymbol{\Sigma}, \tag{3.469}$$

with components $S^i = \frac{1}{2}\epsilon_{ijk}S^{jk}$.

The generator of the pure Lorentz transformations on the right-hand side of (3.467) is also written as $S^{0i} = i\alpha^i/2$ with the matrix

$$\boldsymbol{\alpha} = \begin{pmatrix} -\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \tag{3.470}$$

It is customary to introduce the matrices

$$\sigma^{\mu\nu} \equiv \frac{i}{2}[\gamma^\mu, \gamma^\nu]. \tag{3.471}$$

In terms of these, equations (3.467) can be summarized as

$$S^{\mu\nu} \equiv \frac{1}{2}\sigma^{\mu\nu}. \tag{3.472}$$

It is easy to check that the matrices $S^{\mu\nu}$ satisfy the same commutation rules as the defining generators of the Lorentz group in (3.83):

$$[S^{\mu\nu}, S^{\mu\lambda}] = -ig^{\mu\mu}S^{\nu\lambda}, \quad \text{no sum over } \mu. \tag{3.473}$$

Thus they are generators of a new 4×4 -representation of the Lorentz group. The 4×4 -Dirac representation matrices $D(\Lambda)$ transforming bispinors are mathematically inequivalent to the defining 4×4 -representation Λ of the Lorentz group transforming vectors.

With the gamma matrices, the generators $S^{\mu\nu}$ have the following commutation rules

$$[S^{\mu\nu}, \gamma^\lambda] = -(L^{\mu\nu})^\lambda{}_\kappa \gamma^\kappa = -i(g^{\mu\lambda}\gamma^\nu - g^{\nu\lambda}\gamma^\mu), \tag{3.474}$$

which state that γ^μ is a vector operator in bispinor space [recall (3.93)]. The transformation law (3.462) is the global version of this transformation law.

In terms of the generators $S^{\mu\nu}$, we can write the field transformation law (3.459) more explicitly as

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = D(\Lambda)\psi(\Lambda^{-1}x) = e^{-i\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}\psi(\Lambda^{-1}x), \tag{3.475}$$

As in the case of the scalar field [recall (3.116)], it is useful to perform the transformation of the spacetime argument on the right-hand side in terms of the differential operator of four-dimensional angular momentum and rewrite (3.475) as

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = \hat{D}(\Lambda)D(\Lambda)\psi(x) = e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{J}^{\mu\nu}}\psi(x), \tag{3.476}$$

where

$$\hat{J}^{\lambda\kappa} \equiv S^{\lambda\kappa} \times \hat{1} + 1 \times \hat{L}^{\lambda\kappa}. \tag{3.477}$$

are the generators of the total four-dimensional angular momentum of a Dirac field by analogy with (3.270). The tensor products exhibits the two separate representation spaces associated with Dirac index and spacetime coordinates. The commutation rules between the generators $\hat{J}^{\mu\nu}$ are of course the same as in the case of the vector potential (3.272), and in fact for any spin.

3.13 OTHER SYMMETRIES OF DIRAC ACTION

As in the scalar case, the spin-1/2 action (3.455) is invariant under more than just the Lorentz group.

3.13.1 Translations

First, it is automatically invariant under translations (3.177) for which

$$\psi(x) \longrightarrow \psi'_a(x) = \psi(x-a). \tag{3.478}$$

Together with the Lorentz transformations, these form the *inhomogeneous Lorentz group* or the *Poincaré group* (3.181). Under it, the spinor transforms as

$$\psi(x) \longrightarrow \psi'(x) = \psi(\Lambda^{-1}(x-a)). \tag{3.479}$$

Extending (3.476), we can generate all Poincaré transformations by

$$\psi(x) \xrightarrow{\Lambda} \psi'(x) = \hat{D}(\Lambda)D(\Lambda)\psi(x) = e^{ia^\mu\hat{p}_\mu/\hbar}e^{-i\frac{1}{2}\omega_{\mu\nu}\hat{J}^{\mu\nu}}\psi(x). \tag{3.480}$$

3.13.2 Space Inversion

In contrast to scalar fields, the Ponicaré invariance does not automatically imply invariance under *parity* transformations. In the quantum theory of electrons and photons, quantum electrodynamics (QED), it is an additional requirement confirmed by all experimental data. The action of free electrons must therefore be invariant under parity transformations. To achieve this, we have to first define an appropriate way how to transform a bispinor under space reflections P. The bispinor must form a representation of the Lorentz group extended by P

$$\psi(x) \xrightarrow{P} \psi'_P(x) = D(P)\psi(\tilde{x}), \tag{3.481}$$

where $x'_P = \tilde{x}$ as in (3.187), and the representation matrices $D(P)$ must combine with the representation matrices of the Lorentz group $D(\Lambda)$ in the same way as the 4×4 matrix of space reflections

$$P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \tag{3.482}$$

combines with the Lorentz transformations Λ. From the explicit matrices (3.50)–(3.52) and (3.56)–(3.58) we find

$$P^{-1}\mathbf{L}P = \mathbf{L}, \quad P^{-1}\mathbf{M}P = -\mathbf{M}. \tag{3.483}$$

Thus rotations commute with reflections, which is intuitively obvious since $\mathbf{x}$ and $-\mathbf{x}$ rotate both with the same 3×3 matrices. Pure Lorentz transformations, on the other hand, are space-inverted into those for the opposite direction. Since upper and lower components in a Dirac spinor contain the boost matrices (3.425) in opposite directions, we can immediately write down the transformation law for a Dirac spinor under space inversion as

$$\psi(x) \xrightarrow{P} \psi'_P(x) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \psi(\tilde{x}). \tag{3.484}$$

The phase η_P is the intrinsic parity of the field $\psi(x)$. The representation matrix of the reflection P in Dirac space is denoted by

$$D(P) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \eta_P \gamma_0. \tag{3.485}$$

The property $P^2 = 1$ must be reproduced by the representation matrix $D(P)$. By applying two successive space inversions on $\psi(x)$ we can conclude that the intrinsic parity can only have the values $\eta_P = \pm 1$.

We easily check that the matrix $D(P)$ transforms the 4×4 -bispinor representation (3.467) of the generators L_i and M_i as in the defining representation (3.483):

$$D^{-1}(P)D(L_i)D(P) = D(L_i), \qquad D^{-1}(P)D(M_i)D(P) = D(-M_i). \tag{3.486}$$

We now postulate Lorentz invariance of the action (3.447) under space reflection. Since

$$D^{-1}(P)\begin{pmatrix} M_2 & 0 \\ 0 & M_1 \end{pmatrix} D(P) = \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix}, \tag{3.487}$$

this is only possible if $M_1 = M_2$, so that the action takes the Dirac form (3.455). Also, since space inversion transforms $\xi(x)$ into $\eta(x)$, a parity-invariant theory necessarily contains both fields and thus the full bispinor $\psi(x)$.

Having set $M_1 = M_2$, the mass term of the Dirac action is parity-invariant. In order to ensure the invariance of the derivative term, we observe that the representation matrix (3.485) of P satisfies

$$D^{-1}(P)\gamma^\mu D(P) = \tilde{\gamma}^\mu. \tag{3.488}$$

Hence we calculate

$$\begin{aligned} \bar{\psi}'(x')i\gamma^\mu\partial'_\mu\psi'(x') &= \bar{\psi}'(\tilde{x})i\gamma^\mu\tilde{\partial}_\mu\psi'(\tilde{x}) = \bar{\psi}(x)D^{-1}(P)i\gamma^\mu\tilde{\partial}_\mu D(P)\psi(x) \\ &= \bar{\psi}(x)i\gamma^\mu\partial_\mu\psi(x), \end{aligned} \tag{3.489}$$

which proves the invariance of the derivative term, and thus of the full Dirac action.

The Dirac equation

$$(i\gamma^\mu\partial_\mu - M)\psi(x) = 0$$

can trivially be rewritten as

$$(i\gamma^\mu\tilde{\partial}_\mu - M)\psi(\tilde{x}) = 0.$$

Using (3.484), (3.485) we can replace $\psi(\tilde{x})$ by $\eta_P\gamma_0\psi'_P(x)$, and take the matrix γ_0 to the left of the Dirac operator with the help of (3.488). The result is

$$(i\gamma^\mu\partial_\mu - M)\psi'_P(x) = 0,$$

i.e. the Dirac equation for the mirror-reflected bispinor.

As we shall see in Chapter 10, the interactions of electrons with electromagnetism are described with extreme accuracy by a parity-invariant theory called quantum electrodynamics. The electrons in this theory are described by a Dirac action (3.455).

A theory based only on a single two-component spinor field ξ or η is necessarily massless and violates parity. Such a theory was used successfully to describe *neutrino* processes. There exist several neutrinos in nature, one associated with every charged lepton e^-, μ^-, τ^- whose masses are $m_e = 0.510\,\mathrm{MeV}$, $m_\mu = 105.66\,\mathrm{MeV}$, $m_\tau = 1777.03 \pm 0.30\,\mathrm{MeV}$, the latter two having finite lifetimes $\tau_\mu = (2.19703 \pm 0.00004) \times 10^{-6}\,\mathrm{sec}$ and $\tau_\tau = (290.6 \pm 1.1) \times 10^{-15}\,\mathrm{sec}$. The corresponding neutrinos are denoted by ν_e, ν_μ, ν_τ. The six leptons seem to exist in nature completely parallel to six quarks which are the elemetary buiding blocks of strongly interacting particles. This is illustrated in Fig. 3.1.

FIGURE 3.1 Six leptons and quarks

$$\begin{pmatrix} e^- & \mu^- & \tau^- \\ \nu_e & \nu_\mu & \nu_\tau \end{pmatrix} \qquad \begin{pmatrix} u & c & t \\ d & s & b \end{pmatrix}$$

The electron neutrino was postulated in 1931 by Pauli in order to explain an apparent violation of energy conservation in the final state of the β-decay of the neutron. Energy conservation, would have been violated if only the observed particles proton and electron emerged from the decay. From the energy spectrum of the electron one can deduce that the mass of the electron neutrino is extremely small, less than 2 eV/c^2. The most precise value is expected from an ongoing experiment performed in Karlsruhe. There one studies the beta radiation of tritium which decay in 12.3 years with a total energy release of 18.6 keV shared by elektron and neutrino. The energy of the electrons is measured in KATRIN, a giant electrostatic Spektrometer of 7 m diameter and 20 m length, after which their identity is proved in a semiconducting detector. The experiment is sensitive to electron neutrino masses $\geq 0.4\,\mathrm{eV}/c^2$. The masses of the other two neutrinos have presently the bounds $m_{\nu_\mu} < 0.19\,\mathrm{MeV}$ and $m_{\nu_\tau} < 0.18.3\,\mathrm{MeV}$.

In summary, in a mirror symmetric Lorentz-invariant theory of particles with the lowest nontrivial spin 1/2, the action is given by Dirac's expression (3.455). If parity is allowed to be violated, there are two simpler Lorentz-invariant actions of massless particles

$$\mathcal{A} = \int d^4x\, \mathcal{L}(x) = \int d^4x\, \xi^\dagger(x) i\tilde{\sigma}^\mu \partial_\mu \xi(x), \tag{3.490}$$

or

$$\mathcal{A} = \int d^4x\, \mathcal{L}(x) = \int d^4x\, \eta^\dagger(x) i\sigma^\mu \partial_\mu \eta(x). \tag{3.491}$$

The parity-invariant action (3.455) is the correct one for electrons, the action (3.490) describes neutrinos. For neutrinos, it has become customary to work also with four-component bispinors $\psi(x)$, but make use only of the two upper components of it. The upper and lower components are extracted from $\psi(x)$ by the projection matrices

$$P_{u,l} \equiv \frac{1}{2}(1 \mp \gamma_5) \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.492}$$

where γ_5 denotes the 4×4 -matrix

$$\gamma_5 \equiv i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \gamma^5. \tag{3.493}$$

This is a Lorentz-invariant matrix, since it may also be expressed in the contracted form

$$\gamma_5 = \frac{i}{4!}\epsilon_{\mu\nu\lambda\kappa}\gamma^\mu\gamma^\nu\gamma^\lambda\gamma^\kappa \equiv \gamma^5, \tag{3.494}$$

where $\epsilon_{\mu\nu\lambda\kappa}$ is the completely antisymmetric tensor with $\epsilon_{0123} = 1$. Using γ_5, the actions (3.490), (3.491) can be written as

$$\mathcal{A} = \int d^4x\, \mathcal{L}(x) = \frac{1}{2}\int d^4x\, \bar{\psi}(x) i\gamma^\mu \partial_\mu (1 \mp \gamma_5)\psi(x). \tag{3.495}$$

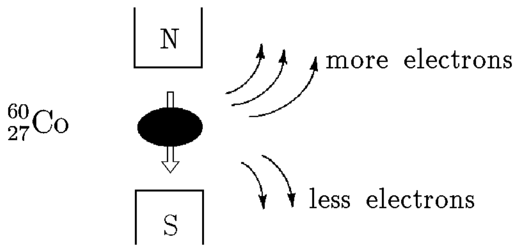

FIGURE 3.2 Asymmetry observed in the distribution of electrons from the β-decay of polarized $^{60}_{27}$Co.

From (3.488) we see that under space inversion, γ_5 transforms as follows:

$$D^{-1}(P)\gamma_5 D(P) = -\gamma_5, \tag{3.496}$$

thereby interchanging the two actions (3.495) with each other.

The parity-violating actions (3.490) and (3.491), or (3.495), have an interesting history. They were first proposed by H. Weyl[11] in 1929 to describe massless spin-1/2 fields, but rejected on theoretical grounds, since at that time all interactions were firmly believed to be invariant under space reflections. Electromagnetic and nuclear interactions had definitely displayed this property, and it was suggestive to assume that nature should follow the same principle in all its interactions. In 1956, however, Lee and Yang pointed out that the decay modes of the heavy mesons K^0 and K^+, the first decaying into $\pi^0\pi^0$ with relative s-waves, the second into $\pi^+\pi^+\pi^-$ with both $\pi^+\pi^+$ and $\pi^-\pi^+$ in relative s-waves, suggested a violation of parity. In 1957, the same authors stressed the relevance of measuring the β-decay from a polarized nucleus.[12] If parity was an invariance of the weak interactions, the distribution of electrons would have to be symmetric with respect to the direction of spin. Indeed, since the scalar product between the spin, which is an axial vector, and the momentum vector is a pseudoscalar operator, its expectation value should vanish. In 1957, Madame Wu and collaborators[13] performed the historic experiment observing a nonzero up-down asymmetry in the distribution of electrons coming from polarized $^{60}_{27}$Co (see Fig. 3.2).[14] The polarization of the sample was done by placing it into a strong magnetic field. By going to a very low temperature, sufficient population difference between spin down and spin up was achieved. The experiment showed a clear violation of parity. In later experiments it was found that the violation is even *maximal*, in the sense that the unobserved neutrino emitted in the decay process can only have one polarization along its momentum direction, the other being *completely* forbidden. A massless neutrino possesses no mirror image in nature and can be described by a pure Weyl action with only a $\frac{1}{2}(1-\gamma_5)\psi$ field. We shall see in the Chapter 5 that also a massless antineutrino is described by the field $\frac{1}{2}(1-\gamma_5)\psi$.

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[11] H. Weyl, J. Phys. *50*, 330 (1929).

[12] T.D. Lee and C.N. Yang, Phys. Rev. *104*, 254 (1956); *105*, 167(1957).

[13] C.S. Wu et al, Phys. Rev. *105*, 1413 (1957).

[14] In nuclear physics the customary notation for a nucleus X is $^A_Z\mathrm{X}_N$, where A is the *nucleon number*, Z the number of protons or *atomic number* (also the *charge number*), and N the number of neutrons. The latter two labels are not necessary for uniqueness since the name of the nucleus is associated with a unique Z, and since $N = A - Z$. They are, however, convenient reminders.

The initial $^{60}_{27}$Co-state has a spin $s=5$ and intrinsic parity $\eta_P=+1$, thus being a $s^P=5^+$-state. The β-decay transforms it into an excited state of $^{60}_{28}$Ni with spin-parity $s^P=4^+$. As such, it is a so-called *Gamow-Teller transition.* In this transition it can be shown that only combinations of tensor and axialvector couplings contribute (T-A). The details will be explained in Chapter 24.

A year later a crucial hypothesis was made by several authors[15] that the weak interactions are mediated by a specific combination of vector and axial vector couplings. This is the famous *V-A hypothesis* which eventually led to the present standard model of weak and electromagnetic interactions (see Chapter 24).

The bispinors $\frac{1}{2}(1\mp\gamma^5)\psi$ are eigenvalues of the matrix γ^5 with eigenvalue ∓ 1. They are called states of left and right *chirality*, respectively.

There exist, of course, many equivalent representations of the Lorentz group including space inversion on spin-1/2 fields including space inversion. Instead of the bispinors $\psi(x)$ transforming with the 4×4 -matrices (3.461), in which h parity exchanges upper and lower two-component spinors in $\psi(x)$ via the matrix $D(P)$ of (3.485), consider symmetric and antisymmetric combinations

$$\psi_{\rm D}(x)\equiv S_{\rm D}\psi(x), \tag{3.497}$$

where $S_{\rm D}$ is the similarity transformation matrix

$$S_{\rm D}\equiv\frac{1}{\sqrt{2}}\left(\begin{array}{rr}1 & 1\\ -1 & 1\end{array}\right). \tag{3.498}$$

In the bispinor $\psi_{\rm D}(x)$, upper and lower components are eigenstates of opposite parity. These fields transform according to the 4×4 representation

$$\begin{aligned} D_{\rm D}(\Lambda) &= S_{\rm D}D(\Lambda)S_{\rm D}^{-1}\\ &= \left(\begin{array}{cc} \frac{1}{2}\left(D^{(\frac{1}{2},0)}+D^{(0,\frac{1}{2})}\right)(\Lambda) & -\frac{1}{2}\left(D^{(\frac{1}{2},0)}-D^{(0,\frac{1}{2})}\right)(\Lambda)\\ -\frac{1}{2}\left(D^{(\frac{1}{2},0)}-D^{(0,\frac{1}{2})}\right)(\Lambda) & \frac{1}{2}\left(D^{(\frac{1}{2},0)}+D^{(0,\frac{1}{2})}\right)(\Lambda)\end{array}\right). \end{aligned} \tag{3.499}$$

When boosting a massive particle from rest to momentum p^μ this matrix becomes explicitly, with (3.425) and (3.422),

$$D_{\rm D}(B_{\hat{\boldsymbol\zeta}}(\zeta)) = \left(\begin{array}{cc} \frac{1}{2}\left(e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}+e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}\right) & -\frac{1}{2}\left(e^{-\boldsymbol{\zeta}\boldsymbol{\sigma}/2}-e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}\right)\\ -\frac{1}{2}\left(e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}-e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}\right) & \frac{1}{2}\left(e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}+e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}\right)\end{array}\right)$$

---

[15] E.C.G. Sudarshan and R.E. Marshak, Phys. Rev. *109*, 1860 (1958); R.P. Feynman and M. Gell-Mann, ibid. 193 (1958); J.J. Sakurai, Nuovo Cimento *7*, 649 (1958); W.R. Theis, Z. Phys. *150*, 590 (1958); Fortschr. Physik *7*, 559 (1959).

$$
\begin{aligned}
&= \begin{pmatrix} \frac{1}{2}\left(\sqrt{p\sigma/M}+\sqrt{p\tilde{\sigma}/M}\right) & -\frac{1}{2}\left(\sqrt{p\sigma/M}-\sqrt{p\tilde{\sigma}/M}\right) \\ -\frac{1}{2}\left(\sqrt{p\sigma/M}-\sqrt{p\tilde{\sigma}/M}\right) & \frac{1}{2}\left(\sqrt{p\sigma/M}+\sqrt{p\tilde{\sigma}/M}\right) \end{pmatrix} \\
&= \frac{1}{\sqrt{2M(M+p_0)}}\begin{pmatrix} M+p_0 & \mathbf{p}\cdot\boldsymbol{\sigma} \\ \mathbf{p}\cdot\boldsymbol{\sigma} & M+p_0 \end{pmatrix}. \qquad (3.500)
\end{aligned}
$$

The Dirac matrices which ensure in this case the invariance of the action (3.447) are now

$$
\gamma^\mu_{\rm D} = S_{\rm D}\gamma^\mu S_{\rm D}^{-1} = \left\{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}\right\}, \qquad (3.501)
$$

$$
\gamma^5_{\rm D} = S_{\rm D}\gamma^5 S_{\rm D}^{-1} = i\gamma^0_{\rm D}\gamma^1_{\rm D}\gamma^2_{\rm D}\gamma^3_{\rm D} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \qquad (3.502)
$$

In terms of these, the boost transformation (3.500) takes the form

$$
D_{\rm D}(B) = \frac{M + \not{p}_{\rm D}\gamma^0_{\rm D}}{\sqrt{2M(p_0+M)}}, \qquad (3.503)
$$

which is the same as the similarity-transformed $S_{\rm D}D(B)S_{\rm D}^{-1}$ of the boost matrix (3.465) in the chiral representation. The generators are

$$
S^{ij}_{\rm D} = S_{\rm D}S^{ij}S_{\rm D}^{-1} = \epsilon_{ijk}\,\frac{1}{2}\begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix}, \quad S^{0i}_{\rm D} = S_{\rm D}S^{0i}S_{\rm D}^{-1} = \frac{i}{2}\begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \qquad (3.504)
$$

which are equal to

$$
\sigma^{\mu\nu}_{\rm D} \equiv S_{\rm D}\sigma^{\mu\nu}S_{\rm D}^{-1} = \frac{i}{2}[\gamma^\mu_{\rm D},\gamma^\nu_{\rm D}], \qquad (3.505)
$$

as in (3.471). The generator of rotations $S^{ij}_{\rm D}$ are the same as in the chiral representation (3.467). Indeed, writing $S^{ij}_{\rm D} = \epsilon_{ijk}\,\frac{1}{2}\,\Sigma^i_{\rm D}$, we see that the 4×4 -generalization of the Pauli matrices (3.468) is invariant under the similarity transformation $S_{\rm D}$:

$$
\boldsymbol{\Sigma}_{\rm D} = S_{\rm D}\boldsymbol{\Sigma}S_{\rm D}^{-1} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} = \boldsymbol{\Sigma}, \qquad (3.506)
$$

so that we can write $S^{ij}_{\rm D} = \epsilon_{ijk}\,\frac{1}{2}\,\Sigma^i$, as before in Eq. (3.469).

For small momenta, the boost matrix (3.500) has the limit

$$
D_{\rm D}(B_{\hat{\mathbf{p}}}(|\mathbf{p}|)) \approx \begin{pmatrix} 1 & \mathbf{p}\cdot\boldsymbol{\sigma}/2 \\ \mathbf{p}\cdot\boldsymbol{\sigma}/2 & 1 \end{pmatrix}. \qquad (3.507)
$$

This shows the spinors in Dirac's representation of the gamma matrices have small lower (or upper) components for slow particles (or antiparticles). The Dirac representation is therefore useful for studying the nonrelativistic limit of Dirac particles.

For such calculations it is useful to state the Dirac matrices in a direct-product form

$$\gamma^0_{\rm D} = \sigma^3 \times 1, \quad \boldsymbol{\gamma}_{\rm D} = i\sigma^2 \times \boldsymbol{\sigma}, \tag{3.508}$$

in which $\gamma_5 = \sigma^1 \times 1$ and the generators of the Lorentz group (3.505) take the form

$$\sigma^{ij}_{\rm D} = \epsilon_{ijk}\Sigma^k = \epsilon_{ijk}\, 1 \times \sigma^k, \quad \sigma^{0i}_{\rm D} = i\sigma^1 \times \sigma^i. \tag{3.509}$$

In each case, the second matrix acts on the up and down components of the spin, the first matrix mixes upper and lower components.

Actually, it is this representation of the Dirac matrices which was found by Dirac himself in his original paper.[16] This is why it is used in most textbooks. It is also referred to as the *standard representation*. In the standard representation, the *chirality matrix* γ^5 is not diagonal, as in the previous representation (3.493). To emphasize this property, the 4×4 -matrices (3.448) are called the *chiral representation* of the gamma matrices (also the *Weyl representation*).

As a historical note we mention that Dirac did not find his matrices from group theoretic considerations but by searching for a relativistic Schrödinger equation for an electron which, in contrast to the Klein-Gordon equation contains only a single time derivative, so that there would be no negative-energy solutions. He wanted the time-independent electron field to satisfy the wave equation

$$\hat{H}\psi(\mathbf{x}) = \sqrt{\hat{\mathbf{p}}^2 + M^2}\psi(\mathbf{x}) = E\psi(\mathbf{x}) \tag{3.510}$$

with only the positive square root. Since in relativistic theories energy and momentum appear on equal footing, he searched for a way to take an explicit square root if the result was allowed to be a matrix. Then $\psi(\mathbf{x}, t)$ could consist of several components representing the spin degrees of freedom of the electron. So he made the ansatz

$$\hat{H}_{\rm D}\psi(\mathbf{x}) = (\alpha^i \hat{p}^i + \beta M)\psi(\mathbf{x}) = E\psi(\mathbf{x}), \tag{3.511}$$

with α_i, β being unknown matrices. Then he required that by applying $\hat{H}_{\rm D}$ twice upon $\psi(\mathbf{x})$ should give $(\hat{\mathbf{p}}^2 + M^2)\psi(\mathbf{x}) = E^2\psi(\mathbf{x})$. This led him to the algebraic relations

$$\begin{aligned} \left\{\alpha^i, \alpha^j\right\} &= \delta_{ij}, \\ \left\{\alpha^i, \beta\right\} &= 0, \\ \beta^2 &= 1. \end{aligned} \tag{3.512}$$

He solved these anticommutators with the matrices

$$\beta = \beta_{\rm D} \equiv \gamma^0_{\rm D} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\alpha} = \boldsymbol{\alpha}_{\rm D} \equiv \gamma^0_{\rm D}\boldsymbol{\gamma}_{\rm D} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}. \tag{3.513}$$

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[16] P.A.M. Dirac, Proc. Roy. Soc. A *117*, 610 (1928), A *118*, 351 (1928).

He could of course have solved them just as well in the chiral representation by

$$\beta\equiv\gamma^0,\qquad \boldsymbol{\alpha}\equiv\gamma^0\boldsymbol{\gamma}=\left(\begin{array}{cc}-\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{array}\right). \tag{3.514}$$

By multiplying Eq. (3.511) with β and going over to a time-dependent equation by replacing E by $\hat{p}_0=i\partial_{x^0}$, he obtained the Dirac equation in the form

$$(\gamma_{\rm D}^{\mu}\hat{p}_{\mu}-M)\psi(x)=0. \tag{3.515}$$

with the matrices

$$\gamma_{\rm D}^{0}\equiv\beta,\qquad \gamma_{\rm D}^{i}\equiv\beta\alpha^{i}. \tag{3.516}$$

The anticommutation relations (3.512) go over into the anticommutation relations (3.450) for the Dirac matrices

$$\{\gamma_{\rm D}^{\mu},\gamma_{\rm D}^{\nu}\}=2g^{\mu\nu}. \tag{3.517}$$

Inserting into the Dirac equation (3.515) the decomposition (3.446) of $\psi(x)$ into the two-component spinors $\xi(x)$ and $\eta(x)$, we find the two equations

$$i\partial_t\xi(x)+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\eta(x) = M\,\xi(x), \tag{3.518}$$

$$i\partial_t\eta(x)+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\xi(x) = -M\,\eta(x). \tag{3.519}$$

to be compared with the equations (3.440) in the chiral representation for $M_1=M_2=M$:

$$\begin{aligned}i\partial_t\xi(x)-i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\xi(x) &= M\,\xi(x),\\ i\partial_t\eta(x)+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\eta(x) &= M\,\eta(x).\end{aligned} \tag{3.520}$$

We have noted before when calculating the small-momentum limit (3.507) that the Dirac representation is most convenient for studying the nonrelativistic limit. This limit, in which $Mc^2\to\infty$, corresponds in natural units to letting $M\to\infty$. The energies of slowly moving particle are very close to M, so that $(i\partial_t-M)\chi(x)$ is much smaller than $(i\partial_t+M)\eta(x)$, which can be approximated by $2M\eta(x)$. The lower equation in (3.519) can therefore be solved approximately by the relation between lower and upper spinor

$$\eta(x)\approx -i\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}}{2M}\xi(x). \tag{3.521}$$

We can also remove the fast temporal oscillations as in (3.151) and replace

$$\left(\begin{array}{c}\xi(x)\\ \eta(x)\end{array}\right)\to e^{-iMc^2t/\hbar}\frac{1}{\sqrt{2M}}\left(\begin{array}{c}\Psi(x)\\ \Phi(x)\end{array}\right). \tag{3.522}$$

If we solve again the lower equation by a relation like (3.521), the upper equation reduces to the Schrödinger equation for each spinor component:

$$i\partial_t\Psi(x)=-\frac{1}{2M}(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})^2\Psi(x). \tag{3.523}$$

Using

$$(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})^2=\sigma^i\sigma^j\nabla_i\nabla_j=\left[\delta^{ij}+i\epsilon_{ijk}\sigma^k\right]\nabla_i\nabla_j=\boldsymbol{\nabla}^2, \tag{3.524}$$

this becomes

$$i\partial_t\Psi(x)=-\frac{1}{2M}\boldsymbol{\nabla}^2\Psi(x). \tag{3.525}$$

In the presence of electromagnetic interactions, the last step will be nontrivial. yielding the nonrelativistic Pauli equation (4.59) with the correct magnetic moment of a Dirac particle.

In both representations, we can insert one equation into the other and find that $\xi(x)$ and $\eta(x)$ satisfy the Klein-Gordon equations (3.441) with $M_1=M_2=M$:

$$\begin{aligned}(-\partial^2-M^2)\xi(x) &= 0,\\ (-\partial^2-M^2)\eta(x) &= 0.\end{aligned} \tag{3.526}$$

This follows of course simply from the Dirac equation (3.454) upon multiplying it by $(i\not{\partial}+M)$and working out

$$(i\not{\partial}+M)\,(i\not{\partial}-M)\,\psi(x)=\left(-\not{\partial}^{\,2}-M^2\right)\psi(x)=\left(-\partial^2-M^2\right)\psi(x). \tag{3.527}$$

In the massless case, the Dirac equations (3.518) and (3.519) have a very similar structure to Maxwells equations (3.237) and (3.238):

$$\begin{aligned}\partial_t\mathbf{B}+\boldsymbol{\nabla}\times\mathbf{E} &= 0,\\ \partial_t\mathbf{E}-\boldsymbol{\nabla}\times\mathbf{B} &= 0.\end{aligned} \tag{3.528}$$

To see this similarity we rewrite the cross product with the help of the 3×3 - generators (3.53) of the rotation group, $(L_i)_{jk}=-i\epsilon_{ijk}$, where they read

$$\begin{aligned}i\partial_t\mathbf{E}+i(\mathbf{L}\cdot\boldsymbol{\nabla})\,(i\mathbf{B}) &= 0,\\ i\partial_t(i\mathbf{B})+i(\mathbf{L}\cdot\boldsymbol{\nabla})\,\mathbf{E} &= 0.\end{aligned} \tag{3.529}$$

The reader is encouraged to discuss the analogy between the transformation properties of (ξ,η) and $(\mathbf{E},i\mathbf{B})$ and the generators $\boldsymbol{\sigma}$ and $\mathbf{L}$.

3.13.3 Charge Conjugation

In Section 3.5.4 we observed that the action of a scalar field was invariant under an extra discrete symmetry not related to the Lorentz group, charge conjugation. It consisted in a simple exchange of the scalar field by its complex conjugate. A similar invariance can be found for the action of the Dirac field. There is only one complication: We must make sure that this operation commutes with the Lorentz group. Thus we must form linear combinations of the components of the conjugate bispinor $\psi^*(x)$ which transform again like the original bispinor $\psi(x)$. Let us call this new bispinor

$$\psi^c(x)\equiv C\bar{\psi}^T(x), \tag{3.530}$$

where the superscript T on the right-hand side indicates a transposition of the row vector $\bar{\psi}$, which makes ψ^c. a column vector. The operation of charge conjugation is then defined by

$$\psi(x) \xrightarrow{C} \psi'_C(x) = \eta_C \psi^c(x), \tag{3.531}$$

with a phase

$$\eta_C = \pm 1. \tag{3.532}$$

The matrix C is determined by the requirement that $\psi'_C(x)$ must satisfy the Dirac equation

$$(i\partial\!\!\!/ - M)\psi'_C(x) = 0. \tag{3.533}$$

Inserting the right-hand side of (3.531) this reads

$$(i\partial\!\!\!/ - M)C\bar{\psi}^T(x) = 0, \tag{3.534}$$

or

$$[iC^{-1}\gamma^\mu C\partial_\mu - M]\bar{\psi}^T(x) = 0. \tag{3.535}$$

The transpose of this is

$$\bar{\psi}(x)[i(C^{-1}\gamma^\mu C)^T \overset{\leftarrow}{\partial}_\mu - M] = 0. \tag{3.536}$$

Consider, on the another hand, the adjoint of the Dirac equation

$$(i\gamma^\mu\partial_\mu - M)\psi(x) = 0, \tag{3.537}$$

which is

$$\psi^\dagger(x)(-i\gamma^{\mu\dagger} \overset{\leftarrow}{\partial}_\mu - M) = 0. \tag{3.538}$$

Multiplying this by γ^0 from the right and using the fact that

$$(\gamma_0)^{-1}\gamma^{\mu\dagger}\gamma^0 = \gamma^\mu, \tag{3.539}$$

we see that

$$\bar{\psi}(x)(-i\gamma^\mu \overset{\leftarrow}{\partial}_\mu - M) = 0. \tag{3.540}$$

Comparing this with (3.536) we conclude that $\psi'_T(x)$ satisfies the Dirac equation if the matrix C satisfies

$$C^{-1}\gamma^\mu C = -\gamma^{\mu T}. \tag{3.541}$$

In both the chiral and the Dirac representation, the transposition of γ^μ changes only the sign of γ^2. A matrix C with this property in the chiral representation is given by

$$C = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix}, \tag{3.542}$$

where c is the 2×2 matrix

$$c = -i\sigma^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{3.543}$$

This matrix is the two-dimensional representation of rotation around the 2-axis by an angle π:

$$c = e^{-i\pi\sigma^2/2}, \tag{3.544}$$

as can esily be verified using (3.411) [or by a direct power series expansion as in (3.410)]. From this rotation property it follows directly [or via Lie's expansion formula (3.99) as in (3.432)] that

$$c^{-1} \begin{pmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{pmatrix} c = \begin{pmatrix} -\sigma^1 \\ \sigma^2 \\ -\sigma^3 \end{pmatrix}, \tag{3.545}$$

and we find

$$\begin{aligned} \begin{pmatrix} c^{-1} & 0 \\ 0 & -c^{-1} \end{pmatrix} \begin{pmatrix} 0 & \sigma^\mu \\ \tilde{\sigma}^\mu & 0 \end{pmatrix} \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} &= \begin{pmatrix} 0 & -c^{-1}\sigma^\mu c \\ -c^{-1}\tilde{\sigma}^\mu c & 0 \end{pmatrix} \\ &= (-\gamma^0, \gamma^1, -\gamma^2, \gamma^3) = -\gamma^{\mu T}, \end{aligned} \tag{3.546}$$

so that (3.541) is fulfilled.

Note that the 2×2 -matrix c satisfies the identities

$$c = -c^T = -c^{-1} = -c^\dagger, \tag{3.547}$$

which also hold for the 4×4 -matrices C:

$$C = C^* = -C^T = -C^{-1} = -C^\dagger. \tag{3.548}$$

Using these proeprties, we find that the conjugate Dirac field behaves under the transformation (3.531) as

$$\bar{\psi}(x) \xrightarrow{C} \bar{\psi}'_C(x) = -\eta_C^* \bar{\psi}^c(x), \tag{3.549}$$

with

$$\bar{\psi}^c(x) \equiv \psi^T(x) C. \tag{3.550}$$

This follows from the simple calculation:

$$\bar{\psi} = \psi^{*T}\gamma^0 \to (C\bar{\psi}^T)^{*T}\gamma^0 = (C\gamma^{0T}\psi^*)^{*T}\gamma^0 = \psi^T\gamma^0 C^T\gamma^0 = -\psi^T C = -\bar{\psi}^c. \tag{3.551}$$

Note that

$$\bar{\psi}^c(x) = \overline{\psi^c}(x), \tag{3.552}$$

since

$$\bar{\psi}^c = \psi^{c\dagger}\gamma^0 = (C\bar{\psi}^T)^\dagger\gamma^0 = (\bar{\psi}^T)^\dagger C^\dagger\gamma^0 = (\psi^\dagger\gamma^0)^{T\dagger} C^\dagger\gamma^0 = \psi^T\gamma^{0T\dagger} C^\dagger\gamma^0 = \psi^T C. \tag{3.553}$$

The minus sign on the right-hand side of Eq. (3.549) will be seen in Chapter 5 to have the important consequence that antiparticles have the opposite intrinsic parity of particles.

By writing the charge conjugation matrix (3.542) as

$$C = i\gamma^0\gamma^2, \tag{3.554}$$

we can take the result directly to the Dirac representation (3.501) where[17]

$$C_{\rm D} \equiv -i\gamma^0_{\rm D}\gamma^2_{\rm D} = -S_{\rm D}\begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} S_{\rm D}^{-1} = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}. \tag{3.555}$$

The reason for the name charge conjugation is the same as in the scalar case. In contrast to the scalar case, however, this cannot simply be seen by studying the effect of charge conjugation upon the conserved particle current. In contrast to Eq. (3.221) which shows that the current reverses its sign under charge conjugation, the operation (3.530) with C satisfying (3.541) leaves the current density (3.456) unchanged:

$$j^\mu(x) \xrightarrow{C} j^{\mu\prime}(x) = j^\mu(x). \tag{3.556}$$

This follows directly from

$$\begin{aligned} j^\mu(x) &= \bar\psi(x)\gamma^\mu\psi(x) \xrightarrow{C} -\psi^T(x)C^{-1}\gamma^\mu C\bar\psi^T(x) \\ &= \psi^T(x)\gamma^{\mu T}\bar\psi^T(x) = \bar\psi(x)\gamma^\mu\psi(x) = j^\mu(x) \end{aligned} \tag{3.557}$$

The proper physical effect will only be reached after field quantization. This makes the fields anticommuting fermion operators which produce a sign change in the last step of the transformation (3.557), thus justifying the name charge conjugation for the operation (3.530).

It is possible to imitate this effect of quantization at the classical level by imagining the classical fields to be *anticommuting* of *Grassmann* variables, Such fields will be introduced in Chapter 10 and used in Chapter 23.

3.13.4 Time Reversal

Let us now see how time reversal acts upon the Dirac field. Under time reversal, the direction of a particle momentum and angular momentum are both reversed, and the generators of the Lorentz group are subject to an automorphism (3.126). The same automorphism is now applied to the 4 × 4 bispinor representation $D(T)$. Writing $D(T) = \eta_T D_T$ we must have

$$D_T^{-1}D(L_i)D_T = -D(L_i)^*, \quad D_T^{-1}D(M_i)D_T = -D(M_i)^*. \tag{3.558}$$

The explicit form of the transformation matrix D_T is now determined by the requirement that the time-reversed field $\psi'_T(x)$ defined by

$$\psi(x) \xrightarrow{T} \psi'_T(x) = D(T)\psi^*(x_T), \tag{3.559}$$

---

[17] The minus sign is added to agree with Dirac's sign convention for $C_{\rm D}$.

with $x_T = -\tilde{x}$, satisfies the Dirac equation

$$(i\gamma^\mu\partial_\mu - M)\psi_T'^{\,*}(x) = 0. \tag{3.560}$$

The reason for the complex conjugation of the field on the right-hand side of (3.559) was discussed in Subsec. 3.5.3, where ist was shown that the Schrödinger equation for the time-reversed Schrödinger operator carries a complex conjugation [see Eq. (3.214)]. This is needed to keep the energy in the time-dependent phase factor e^{ip^0t} positive for $t \to -t$.

Inserting (3.559) into (3.560) we obtain

$$D^{-1}(T)(i\gamma^\mu\partial_\mu - M)D(T)\psi^*(-\tilde{x}) = 0. \tag{3.561}$$

From the original Dirac equation we know that

$$(-i\tilde{\gamma}^\mu\partial_\mu - M)\psi(-\tilde{x}) = 0, \tag{3.562}$$

or

$$(i\tilde{\gamma}^{\mu *}\partial_\mu - M)\psi^*(-\tilde{x}) = 0. \tag{3.563}$$

To be compatible with (3.561), the matrix $D(T)$ has to satisfy

$$D^{-1}(T)\gamma^{\mu *}D(T) = \tilde{\gamma}^\mu. \tag{3.564}$$

In both the chiral and the Dirac representation, the γ^μ-matrices have the property

$$\gamma^{\mu *} = \tilde{\gamma}^{\mu T}. \tag{3.565}$$

Using the property (3.541), of the matrix C, we can substitute

$$\gamma^{\mu T} = -C\gamma^\mu C^{-1}, \tag{3.566}$$

and the condition (3.564) becomes

$$D^{-1}(T)C\tilde{\gamma}^\mu C^{-1}D(T) = -\tilde{\gamma}^\mu. \tag{3.567}$$

This is satisfied by

$$D(T) = \eta_T C\gamma_5. \tag{3.568}$$

It is easy to verify that this matrix transforms the generators of the Lorentz group for the Dirac spinors (3.472) as required by (3.558):

$$D^{-1}(T)S^{\mu\nu}D(T) = -S^{\mu\nu *}. \tag{3.569}$$

3.13.5 Transformation Properties of Currents

An important role in interacting field theory is played by bilinear combinations of the Dirac field formed with 16 combination of Dirac matrices, collectively called Γ, which all are selfadjoint under the Dirac conjugation (3.449):

$$\bar{\Gamma} = \gamma_0 \Gamma^\dagger \gamma_0. \tag{3.570}$$

These are the scalar, vector, tensor, axialvector, and pseudoscalar matrices

$$\Gamma_S \equiv 1, \quad \Gamma_V^\mu \equiv \gamma^\mu, \quad \Gamma_T^{\mu\nu} \equiv \sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu], \quad \Gamma_A^\mu \equiv \gamma^\mu \gamma_5, \quad \Gamma_P \equiv i\gamma_5, \tag{3.571}$$

which form a so-called *Clifford algebra*. They are used to define corresponding *current densities*. The most important of these is *vector current density*

$$j_V^\mu(x) = \bar{\psi}(x)\gamma^\mu\psi(x), \tag{3.572}$$

which turns out to be the source of electromagnetism (see Chapter 10). By sandwiching the other Γ-matrices between two Dirac fields, one obtains fields which transform under the Lorentz group as scalar, tensor, axialvector, and pseudoscalar fields. For instance,

$$j_A^\mu(x) = \bar{\psi}(x)\gamma^\mu\gamma_5\psi(x) \tag{3.573}$$

is an *axialvector current density* which, together with the vector current, is responsible for weak interactions. The combination

$$j_T^{\mu\nu}(x) = \frac{i}{2}\bar{\psi}(x)[\gamma^\mu, \gamma^\nu]\psi(x) \tag{3.574}$$

is a tensor current related to the current spin density to be introduced in Section 6.9.2. The different possible current densities are shown in Table 3.1, which also lists the behavior of these currents under the discrete transformations T, C, P, and their various combinations.

TABLE 3.1 The transformation properties of various composite fields. We have omitted the phase factors η_P, η_C, η_T. The notation is $j_S = \bar{\psi}\psi$, $j_V^\mu = \bar{\psi}\gamma^\mu\psi$, $j_T^{\mu\nu} = \bar{\psi}\frac{i}{2}[\gamma^\mu, \gamma^\nu]\psi$, $j_A^\mu = \bar{\psi}\gamma^\mu\gamma_5\psi$, $P = \bar{\psi}i\gamma_5\psi$. The wiggle on the tensor field in the table denotes the parity transformation on both indices. In the transformation law for charge conjugation we have inserted the minus sign which will arise only after a second quantization of the Dirac field, as explained after Eq. (3.557).

	$j_S(x)$ $\bar{\psi}\psi$	$j_V(x)$ $\bar{\psi}\gamma^\mu\psi$	$j_T(x)$ $\bar{\psi}\frac{i}{2}[\gamma^\mu, \gamma^\nu]\psi$	$j_A^\mu(\mathrm{x})$ $\bar{\psi}\gamma^\mu\gamma_5\psi$	$j_P(x)$ $\bar{\psi}i\gamma_5\psi$
P	$j_S(\tilde{x})$	$\tilde{j}_V(\tilde{x})$	$\tilde{j}_T(\tilde{x})$	$-\tilde{j}_A(\tilde{x})$	$-j_P(\tilde{x})$
C	$j_S(x)$	$-j_V(x)$	$-j_T(x)$	$j_A(x)$	$j_P(x)$
T	$j_S(-\tilde{x})$	$\tilde{j}_V(\tilde{x})$	$-\tilde{j}_T(-\tilde{x})$	$\tilde{j}_A(-\tilde{x})$	$-j_P(-\tilde{x})$
PCT	$j_S(-x)$	$-j_V(-x)$	$j_T(-x)$	$-j_A(-x)$	$j_P(-x)$

3.14 MAJORANA FIELDS

In the chiral and Dirac representations of γ^μ-matrices used so far, the bispinor fields $\psi(x)$ are necessarily complex since only σ^2 and thus γ^2 is imaginary. whereas $\sigma^0, \sigma^1, \sigma^3$ and thus $\gamma^0, \gamma^1, \gamma^3$ are real. One may then wonder whether the Dirac equation $(i\not\partial - M)\psi(x) = 0$, and thus the Lorentz transformations $e^{-i\omega_{\mu\nu}S^{\mu\nu}}$, necessarily mix real and imaginary parts of a spin-1/2 field. It can easily be seen that this is not so. The complex conjugate Dirac fields are transformed by the 4×4 -representation matrices

$$D^*(\Lambda) = \begin{pmatrix} D^{(\frac{1}{2},0)*} & 0 \\ 0 & D^{(0,\frac{1}{2})*} \end{pmatrix}. \tag{3.575}$$

As far as rotations are concerned, $D^{(\frac{1}{2},0)*}$ and $D^{(0,\frac{1}{2})*}$ are equivalent to the original representations by a similarity transformation

$$\begin{aligned} D^{(\frac{1}{2},0)*} &= c^{-1}D^{(\frac{1}{2},0)}c, \\ D^{(0,\frac{1}{2})*} &= c^{-1}D^{(0,\frac{1}{2})}c, \end{aligned} \tag{3.576}$$

with $c = -i\sigma^2$. This follows directly by writing the 2×2 rotation matrices in the explicit form:

$$\left(e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2}\right)^* = e^{i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}^*/2}. \tag{3.577}$$

The complex conjugation reverses the 1- and 3-components in the exponent, since σ^1, σ^3 are real, while preserving the 1-component, since σ^2 is imaginary. Using (3.545) we see that

$$c^{-1}\boldsymbol{\sigma}c = -\boldsymbol{\sigma}^*, \tag{3.578}$$

so that the right-hand side of (3.577) becomes

$$e^{i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}^*} = c^{-1}e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2}c, \tag{3.579}$$

which is the same as (3.576). Therefore, the charge conjugate bispinor

$$\psi^c(x) \equiv C\bar{\psi}^T(x) = C\gamma^{0^T}\psi^*(x) = \begin{pmatrix} 0 & -c \\ c & 0 \end{pmatrix}\psi^*(x) \tag{3.580}$$

transforms under rotations just as $\psi(x)$ itself.

Consider now pure Lorentz transformations of the complex-conjugate bispinor $\psi(x)$:

$$\psi^*(x) \xrightarrow{B} \psi^{*\prime}(x') = \begin{pmatrix} e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}^*/2} & 0 \\ 0 & e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}^*/2} \end{pmatrix}\psi^*(x). \tag{3.581}$$

With (3.578), the right-hand side becomes

$$\begin{pmatrix} c^{-1}e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}c & 0 \\ 0 & c^{-1}e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}c \end{pmatrix}\psi^*(x). \tag{3.582}$$

Writing $\psi(x)$ as in (3.446) we see that the upper complex conjugate components $c\xi^*(x)$ transform like the lower components η, whereas the lower components $c\eta^*(x)$ transform like $\xi(x)$. Hence also under Lorentz transformations, $\psi^c(x)$ behaves like ψ, and we can write for the entire proper Lorentz group the transformation law

$$\psi^{c\prime}(\Lambda x) = D(\Lambda)\psi^c(x), \tag{3.583}$$

with the transformation matrix $D(\Lambda)$ satisfying the relation

$$C^{-1}\gamma^{0^{-1}}D^*(\Lambda)\gamma^0 C = C^{-1}\bar{D}(\Lambda)C = D(\Lambda) \tag{3.584}$$

[recalling the definition of Dirac-adjoint matrices (3.449)]. Since ψ and ψ^c both transform in the same way under $D(\Lambda)$ we may form the combinations

$$\begin{aligned} \chi &\equiv \frac{1}{\sqrt{2}}(\psi + \psi^c), \\ \chi' &\equiv \frac{1}{\sqrt{2}i}(\psi - \psi^c), \end{aligned} \tag{3.585}$$

which are separately irreducible representations of the Lorentz group and eigenstates of charge conjugation with charge parity $\pm\eta_C$. Since the original field had 4 complex degrees of freedom, these combinations only can have half as many degrees of freedom, i.e. four real degrees of freedom. Explicitly, the components of the bispinors (3.585) satisfy in the chiral representation the relations

$$\chi_1^* = -\chi_4, \quad \chi_2^* = \chi_3, \tag{3.586}$$

$$\chi_1' = -\chi_4'^*, \quad \chi_2' = \chi_3'^*. \tag{3.587}$$

We may now ask whether there are γ-matrices which make these real degrees of freedom explicit. This would be the case if we would find a representation of the γ-matrices in which $C\gamma^0$ is the unit matrix. Then ψ^c would be equal to ψ^* and the fields χ, χ' would be purely real. Such a representation does indeed exist. It is given by the γ-matrices in the so-called *Majorana representation*:

$$\begin{aligned} \gamma^0_{\rm M} &= \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \quad \gamma^1_{\rm M} = \begin{pmatrix} i\sigma^3 & 0 \\ 0 & i\sigma^3 \end{pmatrix}, \\ \gamma^2_{\rm M} &= \begin{pmatrix} 0 & -\sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \quad \gamma^3_{\rm M} = \begin{pmatrix} -i\sigma^1 & 0 \\ 0 & -i\sigma^1 \end{pmatrix}. \end{aligned} \tag{3.588}$$

They are obtained from γ^μ in the choral representation (3.448) by a similarity transformation

$$\gamma^\mu_{\rm M} = S_{\rm M}\gamma^\mu S_{\rm M}^{-1}, \tag{3.589}$$

with the transformation matrix

$$S_{\rm M} = \frac{1}{4}\begin{pmatrix} 1-\sigma^2 & 1+\sigma^2 \\ 1+\sigma^2 & -1+\sigma^2 \end{pmatrix}. \tag{3.590}$$

The action written with the Majorana matrices $\gamma^\mu_{\rm M}$ is invariant under Lorentz transformations,

$$D_{\rm M}(\Lambda) = S_M D(\Lambda) S_{\rm M}^{-1}. \tag{3.591}$$

In the Majorana representation (3.588), all γ-matrices are purely imaginary, so that the Dirac equation

$$(i\gamma^\mu_{\rm M}\partial_\mu - M)\chi(x) = 0 \tag{3.592}$$

is purely real. The complex conjugate field satisfies the same equation as χ itself.

$$(i\gamma^\mu_{\rm M}\partial_\mu - M)\chi^*(x) = 0. \tag{3.593}$$

A matrix C of complex-conjugation satisfying (3.541) is now given by

$$C_{\rm M} = \gamma^0_{\rm M} = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix} = i \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}. \tag{3.594}$$

In contrast to the other two representations, this is normalized to $C^2_{\rm M} = 1$ rather than $C^2 = -1$, satisfying

$$C = -C^T = C^{-1} = C^\dagger. \tag{3.595}$$

rather than (3.548). This is more convenient here since we want two successive applications of the operations (3.580) to be the identity operation, $(\psi^c)^c = \psi$. This requires $(C\gamma^{0^T})^2 = 1$. In the other two representations of the gamma matrices where C anticommutes with γ^0, this implies $C^2 = -1$. In the Majorana representation where C and γ^0 commute, one has $C^2 = 1$. Note that up to a factor i, the matrix $C_{\rm M}$ happens coincide with $C_{\rm D}$ of Eq. (3.555).

It should be pointed out that $C_{\rm M}$ is not related to C by a similarity transformation $S_{\rm M} C S_{\rm M}^{-1} = i\gamma^0_{\rm M}\gamma^2_{\rm M}$, since $\gamma^\mu_{\rm M}$ does not have the same sign changes under transposition as γ^μ and $\gamma^\mu_{\rm D}$: Whereas $\gamma^{\mu T} = (\gamma^0, -\gamma^1, \gamma^2, -\gamma^3)$ holds also for the Dirac matrices $\gamma^\mu_{\rm D}$, the Majorana matrices satisfy $\gamma^{\mu T}_{\rm M} = (-\gamma^0, \gamma^1, \gamma^2, \gamma^3)$.

According to (3.871), $C\gamma^0$ is equal to the unit matrix, so that

$$\psi^C = \psi^*, \tag{3.596}$$

The bispinors (3.585) reduce to

$$\chi \equiv \frac{1}{\sqrt{2}}(\psi + \psi^*), \quad \chi' \equiv \frac{1}{\sqrt{2}i}(\psi - \psi^*), \tag{3.597}$$

which are now real fields transforming irreducibly under the Lorentz group. They are called *Majorana spinors.*

Under the operation of charge conjugation they transform into themselves

$$\chi(x) \xrightarrow{C} \chi'_C(x) = \eta_C \chi(x) \tag{3.598}$$

with a charge parity $\eta_C = \pm 1$.

Note that between Majorana spinors $\chi(x)$, the quadratic expressions $\bar{\chi}\gamma^\mu_{\rm M}\chi$ and $\bar{\chi}\gamma^\mu_{\rm M}\gamma^\nu_{\rm M}\chi$ are identically zero.

The γ^5-matrix (3.493) has now the form

$$\gamma_{5\,\rm M} = i\gamma^0_{\rm M}\gamma^1_{\rm M}\gamma^2_{\rm M}\gamma^3_{\rm M} = \begin{pmatrix} \sigma^2 & 0 \\ 0 & -\sigma^2 \end{pmatrix} = i\begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} \equiv \gamma^5_{\rm M}. \tag{3.599}$$

3.14.1 Plane-Wave Solutions of Dirac Equation

By analogy with the scalar case we now seek for all plane-wave solutions of the Dirac equation (3.454):

$$(i\partial\!\!\!/ - M)\psi(x) = 0. \tag{3.600}$$

We make an ansatz

$$f_{\mathbf{p}\,s_3}(x) \equiv u(\mathbf{p},s_3)\frac{e^{-ipx}}{\sqrt{Vp^0/M}}, \qquad f^c_{\mathbf{p}\,s_3}(x) \equiv v(\mathbf{p},s_3)\frac{e^{ipx}}{\sqrt{Vp^0/M}}, \tag{3.601}$$

thereby distinuishing as in (3.172) waves with positive and negative frequencies, and allowing for a spin orientation index s_3. Due to the presence of Dirac indices, the solutions will no longer be merely the complex-cojugates of each other, as in (3.145). The superscript of $f^c_{\mathbf{p}\,s_3}(x)$ indicates the appropriate generalization of complex conjugation.

If the wave functions in (3.601) are to solve the Dirac equation (3.600), the bispinors $u(\mathbf{p},s_3)$ and $v(\mathbf{p},s_3)$ in momentum space have to satisfy the Dirac equations in momentum space

$$(p\!\!\!/ - M)u(\mathbf{p},s_3) = 0, \qquad (p\!\!\!/ + M)v(\mathbf{p},s_3) = 0. \tag{3.602}$$

The normalization of these wave functions will be chosen as in the scalar case by requiring the charge (3.168) of these solutions to be of unit size, with the charge density $j^0(x)$ of Eq. (3.456).

In Section 3.4 we have introduced scalar products for solutions of the Klein-Gordon equation (3.170) with the help of the zeroth component of the conserved particle current. This is generalized to the Dirac case by introducing the scalar products

$$\begin{aligned}
(f_{\mathbf{p}'\,s_3'}, f_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\, \bar{f}_{\mathbf{p}'\,s_3'}(\mathbf{x},t)\gamma^0 f_{\mathbf{p}\,s_3}(\mathbf{x},t) = \delta_{\mathbf{p}',\mathbf{p}}\delta_{s_3',s_3},\\
(f^c_{\mathbf{p}'\,s_3'}, f^c_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\, \bar{f}^c_{\mathbf{p}'\,s_3'}(\mathbf{x},t)\gamma^0 f^c_{\mathbf{p}\,s_3}(\mathbf{x},t) = \delta_{\mathbf{p}',\mathbf{p}}\delta_{s_3',s_3},\\
(f^c_{\mathbf{p}'\,s_3'}, f_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\, \bar{f}^c_{\mathbf{p}'\,s_3'}(\mathbf{x},t)\gamma^0 f_{\mathbf{p}\,s_3}(\mathbf{x},t) = 0,\\
(f_{\mathbf{p}'\,s_3'}, f^c_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\, \bar{f}_{\mathbf{p}'\,s_3'}(\mathbf{x},t)\gamma^0 f^c_{\mathbf{p}\,s_3}(\mathbf{x},t) = 0.
\end{aligned} \tag{3.603}$$

From these we deduce the orthonormality conditions for the bispinors:

$$\begin{aligned}
\bar{u}(\mathbf{p},s_3')\gamma^0 u(\mathbf{p},s_3) &= \frac{p^0}{M}\delta_{s_3',s_3}, & \bar{v}(\mathbf{p},s_3')\gamma^0 v(\mathbf{p},s_3) &= \frac{p^0}{M}\delta_{s_3',s_3},\\
\bar{u}(\mathbf{p},s_3')\gamma^0 v(-\mathbf{p},s_3) &= 0, & \bar{v}(-\mathbf{p},s_3')\gamma^0 u(\mathbf{p},s_3) &= 0.
\end{aligned} \tag{3.604}$$

The reversal of the momentum in $v(-\mathbf{p},s_3)$ appears in the second line since the spatial integrals in (3.604) enforce opposite momenta in scalar products between solutions of positive and negative frequency. According to this, vanishing scalar products in bispinor space are necessary to produce orthogonality.

In contrast to the scalar product (3.170) for Klein-Gordon wave functions, both positive- and negative-frequency solutions have now a positive charge, since for any spinor $\bar{\psi}(x)\gamma^0\psi(x) = \psi^\dagger(x)\psi(x)$ is positive definite.

The explicit form of the bispinors $u(\mathbf{p})$ and $v(\mathbf{p})$ depends on the representation employed for the matrices γ^μ, and we shall discuss the different cases separately.

In an infinite volume we shall use plane wave functions analogous to (3.173):

$$\mathrm{f}_{\mathbf{p}\,s_3}(x) \equiv u(\mathbf{p},s_3)e^{-ipx}, \qquad \mathrm{f}^c_{\mathbf{p}\,s_3}(x) \equiv v(\mathbf{p},s_3)e^{ipx}, \tag{3.605}$$

which satisfy the Lorentz-invariant orthonormality conditions

$$\begin{aligned}
(\mathrm{f}_{\mathbf{p}'s_3'},\mathrm{f}_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\,\bar{\mathrm{f}}_{\mathbf{p}'s_3'}(\mathbf{x},t)\gamma^0\mathrm{f}_{\mathbf{p}\,s_3}(\mathbf{x},t) = 2p^0\,\delta(\mathbf{p}'-\mathbf{p})\delta_{s_3',s_3},\\
(\mathrm{f}^c_{\mathbf{p}'s_3'},\mathrm{f}^c_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\,\bar{\mathrm{f}}^c_{\mathbf{p}'s_3'}(\mathbf{x},t)\gamma^0\mathrm{f}^c_{\mathbf{p}\,s_3}(\mathbf{x},t) = 2p^0\,\delta(\mathbf{p}'-\mathbf{p})\delta_{s_3',s_3},\\
(\mathrm{f}^c_{\mathbf{p}'s_3'},\mathrm{f}_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\,\bar{\mathrm{f}}^c_{\mathbf{p}'s_3'}(\mathbf{x},t)\gamma^0\mathrm{f}_{\mathbf{p}\,s_3}(\mathbf{x},t) = 0,\\
(\mathrm{f}_{\mathbf{p}'s_3'},\mathrm{f}^c_{\mathbf{p}\,s_3})_t &\equiv \int d^3x\,\bar{\mathrm{f}}_{\mathbf{p}'s_3'}(\mathbf{x},t)\gamma^0\mathrm{f}^c_{\mathbf{p}\,s_3}(\mathbf{x},t) = 0.
\end{aligned} \tag{3.606}$$

Spinors in Chiral Representation

Using the chiral representation (3.448) for γ^μ, Eqs. (3.602) take the form

$$\begin{pmatrix} 0 & p\sigma \\ p\tilde{\sigma} & 0 \end{pmatrix} u(\mathbf{p},s_3) = Mu(\mathbf{p},s_3), \qquad \begin{pmatrix} 0 & p\sigma \\ p\tilde{\sigma} & 0 \end{pmatrix} v(\mathbf{p},s_3) = -Mv(\mathbf{p},s_3). \tag{3.607}$$

We can immediately write down 4 × 2 -matrices solving these equations. The first is solved by

$$u(\mathbf{p}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix}, \tag{3.608}$$

the second by

$$v(\mathbf{p}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix}, \tag{3.609}$$

This follows from the matrix identities

$$p\sigma\sqrt{\frac{p\tilde{\sigma}}{M}} \equiv M\sqrt{\frac{p\sigma}{M}}^2\sqrt{\frac{p\tilde{\sigma}}{M}} = M\sqrt{\frac{p\sigma}{M}}\sqrt{\frac{p\sigma}{M}\frac{p\tilde{\sigma}}{M}} \tag{3.610}$$

and

$$p\sigma p\tilde{\sigma} \;=\; \frac{1}{2}(p_\mu p_\nu\sigma^\mu\tilde{\sigma}^\nu + p_\mu p_\nu\tilde{\sigma}^\mu\sigma^\nu) = p_\mu p_\nu = M^2, \tag{3.611}$$

the latter being a direct consequence of (3.443).

The 4×2 -matrices (3.608) and (3.609) can be multiplied by an arbitrary 2×2 -matrix from the right, and they will still solve the equations (3.607). There are several convenient choices for auch a matrix with different advantages, as we shall see below. The two-column vectors in the 4×2 -matrices form independent bispinor solutions of Eqs. (3.607). The projection into these is accomplished by multiplication from the right with two *real* two-component *real* unit spinors, the Pauli spinors (3.401),

$$\chi(\tfrac{1}{2}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi(-\tfrac{1}{2}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.612}$$

By taking the 4×2 -matrices (3.608) as they stand and multiplying them with the unit spinors (3.612), we obtain the *canonical bispinors*

$$u(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix}\chi(s_3). \tag{3.613}$$

The unit spinors (3.612) are eigenvectors of the spin-1/2 generator $L_3 = \sigma^3/2$ of the rotation group:

$$L_3\chi(\tfrac{1}{2}) = \tfrac{1}{2}\chi(\tfrac{1}{2}), \quad L_3\chi(-\tfrac{1}{2}) = -\tfrac{1}{2}\chi(-\tfrac{1}{2}). \tag{3.614}$$

The associated bispinors at rest

$$u(\mathbf{0}, \tfrac{1}{2}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \chi(\frac{1}{2}) \\ \chi(\frac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad u(\mathbf{0}, -\tfrac{1}{2}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \chi(-\frac{1}{2}) \\ \chi(-\frac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}. \tag{3.615}$$

are eigenstates of the 4×4 bispinor representation of the generator of rotations around the z-axis [recall (3.468) (3.472)]:

$$S^3 = S^{12} = \frac{1}{2}\sigma^{12} = \frac{1}{2}\Sigma^3 = \frac{1}{2}\begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}. \tag{3.616}$$

In order to construct explicit bispinors $v(\mathbf{p}, s_3)$ we do not directly multiply them with the unit spinors (3.612) from the right hand side as we did to obtain $u(\mathbf{p}, s_3)$

in (3.613), but use first the above-observed freedon of multiplying (3.609) by an arbitrary 2×2 -matrix from the right. This is necessary to construct a spinor $v(\mathbf{p}, s_3)$ with the physically most appropriate transformation properties unter Lorentz transformations.

It is possible to find from the 4×2 -matrices (3.609) directly the solutions $v(\mathbf{p}, s_3)$ of the second equation in (3.607). We simply define e $v(\mathbf{p}, s_3)$ as the charge conjugate spinor of $v(\mathbf{p}, s_3)$ by an operation of the form (3.530), i.e.,

$$v(\mathbf{p}, s_3) = C\bar{u}^T(\mathbf{p}, s_3). \tag{3.617}$$

It is easy to verify that this $v(\mathbf{p}, s_3)$ solves (3.607). To see this we take

$$\bar{u}(\mathbf{p}, s_3) = u^\dagger(\mathbf{p}, s_3)\gamma^0 = \frac{1}{\sqrt{2}}\chi^\dagger(s_3)\left(\sqrt{\tfrac{p\tilde{\sigma}}{M}} \quad \sqrt{\tfrac{p\sigma}{M}} \right), \tag{3.618}$$

and form

$$\bar{u}^T(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}}^T \\ \sqrt{\frac{p\sigma}{M}}^T \end{pmatrix} \chi^*(s_3). \tag{3.619}$$

Multiplying this by the charge-conjugation matrix C of (3.542) yields

$$C\bar{u}^T(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} c\sqrt{\frac{p\tilde{\sigma}}{M}}^T \\ -c\sqrt{\frac{p\sigma}{M}}^T \end{pmatrix} \chi(s_3), \tag{3.620}$$

with $c = -i\sigma^2$ of Eq. (3.543). At this place we realize that due to the hermiticity property of the Pauli matrices (3.400) and (3.417) one has,

$$\sigma^{\mu *} = \sigma^{\mu T}, \tag{3.621}$$

such that relation (3.578) implies the four-component relation

$$c\sigma^{\mu *}c^{-1} = c\sigma^{\mu T}c^{-1} = \tilde{\sigma}^\mu, \tag{3.622}$$

With this, the charge-conjugate spinor $u^c(\mathbf{p}, s_3) = C\bar{u}^T(\mathbf{p}, s_3)$ goes directly over into the bispinor

$$v(\mathbf{p}, s_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} c\chi^*(s_3), \tag{3.623}$$

Thus, while the 4×2 -solutions $u(\mathbf{p})$ of Eq. (3.608) are multiplied by the Pauli spinors $\chi(s_3)$ of Eq. (3.612), the 4×2 -solutions $v(\mathbf{p})$ of Eq. (3.609) are multiplied from the right by the spinors

$$\chi^c(s_3) \equiv c\chi(s_3) = \chi(-s_3)(-1)^{s-s_3}. \tag{3.624}$$

These are called *charge-conjugate Pauli spinors*. Their explicit form is

$$\chi^c(s_3) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix}. \tag{3.625}$$

This construction is necessary to make sure that the Pauli spinors $v(\mathbf{p}, s_3)$ at rest have the same transformation behavior under rotations as the spinors $u(\mathbf{p}, s_3)$ at rest.

Under a rotation, the original basis spinors $\chi(s_3)$ are multiplied by a 2×2 rotation matrix $e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}$. Then their spin indices are linearly recombined with each other by the rotation matrix as follows:

$$\chi(s_3) \xrightarrow{R} \chi'(s_3) = e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}\chi(s_3) = \sum_{s_3'=-1/2}^{1/2} \chi(s_3') \left(e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}\right)_{s_3,s_3'}. \tag{3.626}$$

The last step follows from the specific form (3.612) of the unit spinors. The same mixing occurs in the charge-conjugate spinors

$$\chi^c(s_3) \xrightarrow{R} \chi'^c(s_3) = c\chi'^*(s_3) = ce^{i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}^*/2}\chi^*(s_3) \tag{3.627}$$

Using (3.578), we see that

$$c^{-1}e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}c = e^{i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}^*/2}, \tag{3.628}$$

such that the right-hand side becomes

$$e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}c\chi^*(s_3) = e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}\chi^c(s_3) = \sum_{s_3'=-1/2}^{1/2} \chi^c(s_3') \left(e^{-i\boldsymbol{\phi}\cdot\boldsymbol{\sigma}/2}\right)_{s_3,s_3'}, \tag{3.629}$$

such that $\chi^c(s_3)$ is indeed rotated prescisely like $\chi(s_3)$.

At rest, the 4 × 2 -matrices (3.608) and (3.609) becomes

$$u(\mathbf{p}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sigma^0 \\ \sigma^0 \end{pmatrix}, \qquad v(\mathbf{p}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sigma^0 \\ -\sigma^0 \end{pmatrix}, \tag{3.630}$$

such that the rotation properties of the bispinors $u(\mathbf{p}, s_3) = u(\mathbf{p})\chi(s_3)$ and $v(\mathbf{p}, s_3) = v(\mathbf{p})\chi^c(s_3)$ at rest are the same as those of $\chi(s_3)$ and $\chi^c(s_3)$.

Explicitly, the bispinors $v(\mathbf{p}, s_3)$ at rest become

$$v(\mathbf{0}, \tfrac{1}{2}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \chi^c(\frac{1}{2}) \\ -\chi^c(\frac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \; v(\mathbf{0}, -\tfrac{1}{2}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \chi^c(-\frac{1}{2}) \\ -\chi^c(-\frac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \tag{3.631}$$

to be compared with (3.615) for $u(\mathbf{0}, s_3)$.

For the bispinors at rest (3.615) and (3.631), the Dirac equations in momentum space (3.602) take the simple form

$$M(\gamma^0 - 1)u(\mathbf{0}, s_3) = 0, \qquad M(\gamma^0 + 1)v(\mathbf{0}, s_3) = 0. \tag{3.632}$$

By applying the boost matrix (3.465), we find the alternative expression for the bispinors with momentum $\mathbf{p}$:

$$u(\mathbf{p}, s_3) = \frac{M + \not{p}\gamma^0}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi(s_3) \\ \chi(s_3) \end{pmatrix}, v(\mathbf{p}, s_3) = \frac{M + \not{p}\gamma^0}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi^c(s_3) \\ -\chi^c(s_3) \end{pmatrix}. \tag{3.633}$$

Since γ^0 is a simple off-diagonal unit matrix, we can replace it by ±1 in the left and right equation, respectively, and write just as well

$$u(\mathbf{p}, s_3) = \frac{M + \not{p}}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi(s_3) \\ \chi(s_3) \end{pmatrix}, v(\mathbf{p}, s_3) = \frac{M - \not{p}}{\sqrt{2M(p_0 + M)}} \frac{1}{\sqrt{2}} \begin{pmatrix} \chi^c(s_3) \\ -\chi^c(s_3) \end{pmatrix}. \tag{3.634}$$

The two sets of bispinors $u(\mathbf{p}, s_3)$ and $v(-\mathbf{p}, s_3)$ satisfy the orthonormality conditions (3.604). Using (3.613) and (3.623), we find

$$\begin{aligned} u^\dagger(\mathbf{p}, s_3)u(\mathbf{p}, s_3') &= \frac{1}{2}\chi^T(s_3) \left(\sqrt{\frac{p\sigma}{M}}, \sqrt{\frac{p\tilde{\sigma}}{M}} \right) \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s_3') \\ &= \chi^T(s_3) \frac{1}{2} \left(\frac{p\sigma}{M} + \frac{p\tilde{\sigma}}{M} \right) \chi(s_3') \\ &= \frac{p^0}{M} \chi^T(s_3)\chi(s_3') = \frac{p^0}{M} \delta_{s_3, s_3'}, \end{aligned} \tag{3.635}$$

$$\begin{aligned} v^\dagger(-\mathbf{p}, s_3)v(-\mathbf{p}, s_3') &= \frac{1}{2}\chi^{cT}(s_3) \left(\sqrt{\frac{p\tilde{\sigma}}{M}}, -\sqrt{\frac{p\sigma}{M}} \right) \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(s_3') \\ &= \frac{p^0}{M} \delta_{s_3 s_3'}, \end{aligned} \tag{3.636}$$

$$\begin{aligned} u^\dagger(\mathbf{p}, s_3)v(-\mathbf{p}, s_3') &= \frac{1}{2}\chi^T(s_3) \left(\sqrt{\frac{p\sigma}{M}}, -\sqrt{\frac{p\tilde{\sigma}}{M}} \right) \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(s_3') \\ &= 0, \end{aligned} \tag{3.637}$$

$$v^\dagger(-\mathbf{p}, s_3)u(\mathbf{p}, s_3') = 0. \tag{3.638}$$

The reason for the appearance of the negative momenta in the bispinors $v(-\mathbf{p}, s_3)$ is that the plane wave solutions $f^c_{\mathbf{p}\,s_3}(x)$ in (3.601) carry negative momenta, so that states of a fixed momentum $\mathbf{p}$ are associated with $f_{\mathbf{p}\,s_3}(x)$ and $f^c_{-\mathbf{p}\,s_3}(x)$. The momentum reversal in the conjugate wave functions goes along with the reversal of the spin orientation in the charge-conjugate Pauli spinors Eq. (3.624). The physical reason for these two reversals will be understood after field quantization in Section 5.3.3.

Inserting a matrix γ^0 between the bispinors in (3.635) (3.638) we may also derive orthonormality relations between bispinors $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$:

$$\begin{aligned} \bar{u}(\mathbf{p}, s_3)u(\mathbf{p}, s_3') &= \delta_{s_3,s_3'}, \\ \bar{v}(\mathbf{p}, s_3)v(\mathbf{p}, s_3') &= -\delta_{s_3,s_3'}, \\ \bar{u}(\mathbf{p}, s_3)v(\mathbf{p}, s_3') &= 0, \\ \bar{v}(\mathbf{p}, s_3)u(\mathbf{p}, s_3') &= 0. \end{aligned} \tag{3.639}$$

The two sets of spinors $u(\mathbf{p}, s_3)$ and $v(-\mathbf{p}, s_3)$ span the spinor space at a fixed momentum. This may be expressed by a completeness relation

$$\sum_{s_3} \Big[u(\mathbf{p}, s_3)u^\dagger(\mathbf{p}, s_3) + v(-\mathbf{p}, s_3)v^\dagger(-\mathbf{p}, s_3)\Big] = \frac{p^0}{M}. \tag{3.640}$$

To prove this 4×4 -matrix equation in Dirac space, we derive the separate polarization sums[18] for u- and v-spinors. These can be calculated directly from (3.613) and (3.623) as follows:

$$\begin{aligned} \sum_{s_3} u(\mathbf{p}, s_3)\bar{u}(\mathbf{p}, s_3) &= \frac{1}{2}\begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \sum_{s_3} \chi(s_3)\chi^\dagger(s_3) \left(\sqrt{\frac{p\tilde{\sigma}}{M}}, \sqrt{\frac{p\sigma}{M}}\right) \\ &= \frac{1}{2}\begin{pmatrix} 1 & \frac{p\sigma}{M} \\ \frac{p\tilde{\sigma}}{M} & 1 \end{pmatrix} = \frac{\not{p} + M}{2M} \end{aligned} \tag{3.641}$$

$$\begin{aligned} \sum_{s_3} v(\mathbf{p}, s_3)\bar{v}(\mathbf{p}, s_3) &= \frac{1}{2}\begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \sum_{s_3} \chi^c(s_3)\chi^{c\dagger}(s_3) \left(-\sqrt{\frac{p\tilde{\sigma}}{M}}, \sqrt{\frac{p\sigma}{M}}\right) \\ &= \frac{1}{2}\begin{pmatrix} -1 & \frac{p\sigma}{M} \\ \frac{p\tilde{\sigma}}{M} & -1 \end{pmatrix} = \frac{\not{p} - M}{2M}. \end{aligned} \tag{3.642}$$

Combining the two polarization sums for $\mathbf{p}$ and $-\mathbf{p}$, respectively, and multiplying them by γ^0 proves their completeness.

By subtracting the two polarization sums from each other yields another completeness relation

$$\sum_{s_3} \left[u(\mathbf{p}, s_3)\bar{u}(\mathbf{p}, s_3) - v(\mathbf{p}, s_3)\bar{v}(\mathbf{p}, s_3)\right] = 1. \tag{3.643}$$

There is a minus sign in the second sum which corresponds to the minus sign in the second orthogonality relation (3.639). This sign will be important in Section 5.8 to prove a famous theorem on the relation bewteen spin and statistics of fundamental particles.

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[18] Since They may be called *semi-completeness relations*.

Polarization sums will frequently be needed later, in particular in the process of field quantization. We introduce the sums

$$P(p) \equiv \sum_{s_3} u(\mathbf{p}, s_3) u^\dagger(\mathbf{p}, s_3), \qquad \bar{P}(p) \equiv \sum_{s_3} v(\mathbf{p}, s_3) v^\dagger(\mathbf{p}, s_3), \tag{3.644}$$

defined only for p^0 on the mass shell, $p^0 = \omega_{\mathbf{p}}$. They satisfy the relation $\bar{P}(p) = -P(-p)$. Similar polarization sums exist for plane-wave solutions for any spin. In general, the polarization sums $P(p)$ and $\bar{P}(p)$ of positive and negative energies of momenta $\mathbf{p}$ and $-\mathbf{p}$, respectively, fulfill the relation

$$\bar{P}(p) = \pm P(-p), \tag{3.645}$$

where the upper sign holds for integer spin, the lower for half-integer spin. The matrices $P(p)$ and $P(-p)$ are projection matrices onto solutions of momenta $\mathbf{p}$ and $-\mathbf{p}$ with energies $p^0 = \omega_{\mathbf{p}}$ and $p^0 = -\omega_{\mathbf{p}}$, respectively. As such they satisfy

$$P(\pm p)^2 = P(\pm p). \tag{3.646}$$

It is always possible to find a single covariant expression for $P(p)$ defined for arbitrary off-shell values of p^0, which at the on-shell values $p^0 = \pm\omega_{\mathbf{p}}$ reduces to th above projections $P(p)$ and $P(-p)$. In the Dirac case, where $P(p) = (\not{p} - M)\gamma^0/2M$, we verify that (3.646) is true for $p^0 = \pm\omega_{\mathbf{p}}$.

Spinors in Dirac Representation

Let us also write down the bispinors in the Dirac representation (3.501) of the γ-matrices. The rest bispinors are solutions of equations (3.632), where

$$\gamma^0_{\rm D} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Thus we have

$$u(\mathbf{0}, \tfrac{1}{2}) = \begin{pmatrix} \chi(\frac{1}{2}) \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u(\mathbf{0}, -\tfrac{1}{2}) = \begin{pmatrix} \chi(-\frac{1}{2}) \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \tag{3.647}$$

and

$$v(\mathbf{0}, \tfrac{1}{2}) = \begin{pmatrix} 0 \\ \chi^c(\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad v(\mathbf{0}, -\tfrac{1}{2}) = \begin{pmatrix} 0 \\ \chi^c(-\frac{1}{2}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}. \tag{3.648}$$

The bispinors at finite momentum are obtained from these by applying the 4 × 4 boost matrix (3.465), yielding

$$u(\mathbf{p},s_3)=\frac{M+\not{p}_{\rm D}}{\sqrt{2M(p_0+M)}}\left(\begin{array}{c}\chi(s_3)\\0\end{array}\right),\quad v(\mathbf{p},s_3)=\frac{M-\not{p}_{\rm D}}{\sqrt{2M(p_0+M)}}\left(\begin{array}{c}0\\\chi^c(s_3)\end{array}\right).\tag{3.649}$$

Since $\gamma_{\rm D}^0$ has a simple diagonal form with eigenvalues ±1 for upper and lower spinor components [see Eq. (3.513)], we have replaced $\gamma_{\rm D}^0$ directly by its eigenvalues when going from (3.465) to (3.649) [as we did from (3.633) to (3.634)]. More explicitly, we can write

$$u(\mathbf{p},s_3)=\left(\begin{array}{c}\sqrt{\frac{p_0+M}{2M}}\\\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\sqrt{2M(p_0+M)}}\end{array}\right)\chi(s_3),\; v(\mathbf{p},s_3)=\left(\begin{array}{c}\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\sqrt{2M(p_0+M)}}\\\sqrt{\frac{p_0+M}{2M}}\end{array}\right)\chi^c(s_3).\tag{3.650}$$

In this representation, the bispinors $u(\mathbf{p},s_3)$ of slowly moving particles have large upper and small lower spinor components. The converse is true for the bispinors $v(\mathbf{p},s_3)$. This is what makes the original Dirac spinors useful for discussing the nonrelativistic limit of spin-1/2 particles, as observed before in the boost matrix (3.507) and in x-space equations (3.520).

The Dirac spinors possess of course the same polarization sums (3.644) as in the chiral case, if the appropriate Dirac matrices $\gamma_{\rm D}^\mu$ are used on the right-hand side.

Helicity Spinors

Sometimes, the choice of the spinors (3.612) with the particle spins quantized along the z-axis will not be the most convenient basis in spinor space. Instead of the z-axis, one may choose any quantization direction, in particular, the direction of the momentum of the particle. This amounts to multiplying the 4 × 2 -matrix solutions (3.608) by a 2 × 2 rotation matrix from the right:

$$R(\hat{\mathbf{p}})\equiv e^{-i\phi\sigma^3/2}e^{-i\theta\sigma^2/2},\tag{3.651}$$

where θ, ϕ are the spherical angles of the momentum $\mathbf{p}$. In contrast to the notation in (3.9), the rotation matrix carries now an argument indicating that the z-direction is rotated into the momentum direction indicated by the unit vector $\hat{\mathbf{p}}$.[19] Equivalently, we may choose in the bispinors (3.613), instead of $\chi(s_3)$, a basis $\chi_h(\hat{\mathbf{p}},\lambda)$ with $\lambda=\pm1/2$, defined by

$$\chi_h(\hat{\mathbf{p}},\lambda)\equiv R(\hat{\mathbf{p}})\,\chi(s_3)\equiv e^{-i\phi\sigma^3/2}e^{-i\theta\sigma^2/2}\chi(\lambda).\tag{3.652}$$

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[19] As before in this chapter, hats on vectors in this section denote unit vectors, not Schrödinger operaters.

Explicitly:

$$\chi_h(\hat{\mathbf{p}},\tfrac{1}{2}) = \left(\begin{array}{c} \cos\dfrac{\theta}{2}\, e^{-i\phi/2} \\ \sin\dfrac{\theta}{2}\, e^{i\phi/2} \end{array} \right), \qquad \chi_h(\hat{\mathbf{p}},-\tfrac{1}{2}) = \left(\begin{array}{c} -\sin\dfrac{\theta}{2}\, e^{-i\phi/2} \\ \cos\dfrac{\theta}{2}\, e^{i\phi/2} \end{array} \right). \tag{3.653}$$

The spinors (3.652) diagonalize the projection of the angular momentum in the rest frame along the direction of motion of the particle $\hat{\mathbf{p}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the so-called *helicity*:

$$h(\hat{\mathbf{p}}) \equiv \mathbf{L}\cdot\hat{\mathbf{p}} = \frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} = \frac{1}{2}\left(\begin{array}{cc} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{array} \right). \tag{3.654}$$

The eigenvalues are

$$h(\mathbf{p})\chi(\hat{\mathbf{p}},\lambda) = \lambda\chi(\hat{\mathbf{p}},h), \quad \lambda = \pm\frac{1}{2}. \tag{3.655}$$

The eigenstates $\chi_h(\hat{\mathbf{p}},\lambda)$ are called *helicity spinors*. The associated bispinors are, as in (3.613) and (3.623),

$$u_h(\mathbf{p},\lambda) = \frac{1}{\sqrt{2}}\left(\begin{array}{c} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{array} \right)\chi(\hat{\mathbf{p}},\lambda), \qquad v_h(\mathbf{p},\lambda) = \frac{1}{\sqrt{2}}\left(\begin{array}{c} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{array} \right)\chi^c(\hat{\mathbf{p}},\lambda), \tag{3.656}$$

with the charge-conjugate helicity spinors

$$\chi^c(\hat{\mathbf{p}},\lambda) = c\chi^*(\hat{\mathbf{p}},\lambda). \tag{3.657}$$

These diagonalize the 4×4 bispinor representation of the helicity:

$$H(\hat{\mathbf{p}}) \equiv \mathbf{S}\cdot\hat{\mathbf{p}} = \frac{1}{2}\boldsymbol{\Sigma}\cdot\hat{\mathbf{p}} = \frac{1}{2}\left(\begin{array}{cc} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{array} \right)\cdot\hat{\mathbf{p}}. \tag{3.658}$$

This is a direct consequence of the fact that $H(\hat{\mathbf{p}})$ commutes with the boost matrix (3.465).

Alternatively, we can obtain the helicity bispinors (3.656) by boosting the bispinors at rest (3.652), (3.653), first into the z-direction, and rotating them afterwards into the $\hat{\mathbf{p}}$ direction

$$u_h(\hat{\mathbf{p}},\lambda) \;=\; \frac{1}{\sqrt{2}}\left(\begin{array}{c} R(\hat{\mathbf{p}})\sqrt{\frac{p^0\sigma^0-|\mathbf{p}|\sigma^3}{M}}\chi(h) \\ R(\hat{\mathbf{p}})\sqrt{\frac{p^0\sigma^0+|\mathbf{p}|\sigma^3}{M}}\chi(h) \end{array} \right), \tag{3.659}$$

and

$$v_h(\hat{\mathbf{p}},\lambda) = \frac{1}{\sqrt{2}}\left(\begin{array}{c} R(\hat{\mathbf{p}})\sqrt{\frac{p^0\sigma^0+|\mathbf{p}|\sigma^3}{M}}\chi^c(h) \\ -R(\hat{\mathbf{p}})\sqrt{\frac{p^0\sigma^0-|\mathbf{p}|\sigma^3}{M}}\chi^c(h) \end{array} \right). \tag{3.660}$$

The equality with (3.656) follows from the transformation law (3.431), according to which

$$R(\hat{\mathbf{p}})|\mathbf{p}|\sigma^3 = \mathbf{p}\cdot\boldsymbol{\sigma}R(\hat{\mathbf{p}}). \tag{3.661}$$

One of the important advantages of the helicity spinor is that it has a smooth limit as the particle mass M tends to zero. Indeed, by expanding

$$p^0 = \sqrt{\mathbf{p}^2 + M^2} = |\mathbf{p}| + \frac{M^2}{2|\mathbf{p}|} + \dots \tag{3.662}$$

we see that

$$\begin{aligned}\frac{p^0\sigma^0 - |\mathbf{p}|\sigma^3}{M} &\xrightarrow{M\to 0} \frac{2}{M}\begin{pmatrix} 0 & 0 \\ 0 & |\mathbf{p}| \end{pmatrix},\\ \frac{p^0\sigma^0 + |\mathbf{p}|\sigma^3}{M} &\xrightarrow{M\to 0} \frac{2}{M}\begin{pmatrix} |\mathbf{p}| & 0 \\ 0 & 0 \end{pmatrix}.\end{aligned} \tag{3.663}$$

Thus the massless helicity spinors $u_h(\mathbf{p},\lambda)$ and $v_h(\mathbf{p},\lambda)$ have only two nonzero components. We shall normalize them to

$$u_h^\dagger(\mathbf{p},\lambda)u(\mathbf{p},\lambda) = 2p^0 = 2|\mathbf{p}|, \qquad v_h^\dagger(\mathbf{p},\lambda)v(\mathbf{p},\lambda) = 2p^0 = 2|\mathbf{p}|, \tag{3.664}$$

as opposed the normalization to p^0/M of the massive spinors (3.656). The explicit form is

$$\begin{aligned} u_h(\mathbf{p},\tfrac{1}{2}) &= \sqrt{|\mathbf{p}|}\begin{pmatrix} 0 \\ 0 \\ R(\hat{\mathbf{p}})\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} \equiv u_R(\mathbf{p}),\\ u_h(\mathbf{p},-\tfrac{1}{2}) &= \sqrt{|\mathbf{p}|}\begin{pmatrix} R(\hat{\mathbf{p}})\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0 \\ 0 \end{pmatrix} \equiv u_L(\mathbf{p}), \end{aligned} \tag{3.665}$$

and

$$\begin{aligned} v_h(\mathbf{p},\tfrac{1}{2}) &= \sqrt{|\mathbf{p}|}\begin{pmatrix} 0 \\ 0 \\ -R(\hat{\mathbf{p}})\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = v_R(\mathbf{p})\\ v_h(\mathbf{p},-\tfrac{1}{2}) &= \sqrt{|\mathbf{p}|}\begin{pmatrix} -R(\hat{\mathbf{p}})\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 \\ 0 \end{pmatrix} = v_L(\mathbf{p}). \end{aligned} \tag{3.666}$$

The helicity bispinors $u_h(\mathbf{p},\lambda)$ and $v_h(\mathbf{p},\lambda)$ are eigenstates of the chirality matrix

$$\gamma_5 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.667}$$

with the eigenvalue 2λ. By applying the 4×4 projection matrix $\frac{1-\gamma_5}{2}$ to the bispinors $u_h(\mathbf{p},\lambda)$, forming

$$\frac{1-\gamma_5}{2}u_h(\mathbf{p},\lambda), \tag{3.668}$$

we obtain a negative helicity state. Such projected bispinors are used for the description of neutrinos which only exist with negative helicity (*left-handed neutrinos*). As we shall see later in Section 24.4, weak interactions involve also the arthogonally projected bispinors

$$\frac{1+\gamma_5}{2}v_h(\mathbf{p},\lambda) \tag{3.669}$$

which describe antineutrinos. These exist only with positive helicity (*right-handed antineutrinos*).

3.15 LORENTZ TRANSFORMATION OF SPINORS

Let us study the behavior of the bispinors $u(\mathbf{p},s_3)$ and $v(\mathbf{p},s_3)$ under Lorentz transformations. This will be most straight-forward in the chiral representation, where we may focus attention upon the upper components only which we shall denote by $\xi(\mathbf{p},s_3)$. The properties of the lower components, to be denoted by $\eta(\mathbf{p},s_3)$, can be obtained by a simple change in the direction of the momentum. The upper components can be written explicitly as

$$\xi(\mathbf{p},s_3) = B_{\hat{\zeta}}(\zeta)\chi(s_3) = e^{-\zeta\cdot\sigma/2}\chi(s_3). \tag{3.670}$$

Applying a general Lorentz transformation $D^{(\frac{1}{2},0)}(\Lambda)$ to this, the momentum $\mathbf{p}$ is changed to some other vector $\mathbf{p}'$, which is the spatial part of the four-vector $\Lambda^{\mu}{}_{\nu}p^{\nu}$. The transformation can be done in three steps: First deboost the particle by applying a boost opposite to the particle's momentum which brings it to rest, with the four-momentum p^{μ} becoming $p^{\mu}_R = (M,\mathbf{0})$. Second we perform a rotation, and third we boost the particle to its final four-momentum p'^{μ}. Thus we can write the general Lorentz transformations as

$$D^{(\frac{1}{2},0)}(\Lambda) = B_{\hat{\zeta}'}(\zeta')W(p',\Lambda,p)B^{-1}_{\hat{\zeta}}(\zeta) \equiv e^{-\zeta'\cdot\sigma/2}e^{-i\alpha\cdot\sigma/2}e^{\zeta\cdot\sigma/2}. \tag{3.671}$$

The rotation $W(p',\Lambda,p)$ in the middle is called a *Wigner rotation*. It is an element of the little group of the massive particle acting only in its rest frame [see the earlier short discussion on p. 114].

Let p' be the momentum reached from the momentum p after a Lorentz transformation Λ. Then the spinor (3.670) changes as follows:

$$\xi(\mathbf{p},s_3) \xrightarrow{\Lambda} \xi'(\mathbf{p}',s_3) \;=\; D^{(\frac{1}{2},0)}(\Lambda)\xi(\mathbf{p},s_3) = e^{-\zeta'\cdot\sigma/2}e^{-i\alpha\cdot\sigma/2}\chi(s_3)$$

$$= e^{-\zeta'\cdot\sigma/2} \sum_{s_3'=-1/2}^{1/2} \chi(s_3') \left(e^{-i\alpha\cdot\sigma/2}\right)_{s_3',s_3}$$

$$= \sum_{s_3'=-1/2}^{1/2} \xi(\mathbf{p}', s_3') W_{s_3',s_3}(p', \Lambda, p), \tag{3.672}$$

where we have used the rotation property (3.626) of the spinors $\chi(s_3)$, which amounts here to

$$W(p', \Lambda, p)\chi(s_3) = \sum_{s_3'=-1/2}^{1/2} \chi(s_3') W_{s_3',s_3}(p', \Lambda, p). \tag{3.673}$$

By analogy, the spinor $\eta(\mathbf{p}, s_3)$ transforms like

$$\eta(\mathbf{p}, s_3) \xrightarrow{\Lambda} \eta'(\mathbf{p}', s_3) = D^{(0,\frac{1}{2})}(\Lambda)\eta(\mathbf{p}, s_3) = \sum_{s_3'=-1/2}^{1/2} \eta(\mathbf{p}', s_3') W_{s_3',s_3}(p', \Lambda, p), \tag{3.674}$$

implying for the Dirac spinor $u(\mathbf{p}, s_3)$ the transformation law

$$u(\mathbf{p}, s_3) \xrightarrow{\Lambda} u'(\mathbf{p}', s_3) = D(\Lambda)u(\mathbf{p}, s_3) = \sum_{s_3'=-1/2}^{1/2} u(\mathbf{p}', s_3') W_{s_3',s_3}(p', \Lambda, p). \tag{3.675}$$

The result can be expressed most compactly in terms of the 4 × 2 -matrix form (3.609) for the bispinor solutions as

$$u(\mathbf{p}) \xrightarrow{\Lambda} u'(\mathbf{p}') = D(\Lambda)u(\mathbf{p}) = u(\mathbf{p}')W(p', \Lambda, p), \tag{3.676}$$

We are now prepared to understand the group-theoretic reason for the occurrence of the rotation matrix $c = e^{-i\pi\sigma_2/2}$ in the charge conjugate bispinor $v(\mathbf{p})$ of Eq. (3.623). The 4 × 2 solutions $v(\mathbf{p})$ of (3.609) transform in the same way as $u(\mathbf{p})$ of (3.608):

$$v(\mathbf{p}) \xrightarrow{\Lambda} v'(\mathbf{p}') = D(\Lambda)v(\mathbf{p}) = v(\mathbf{p}')W(p', \Lambda, p). \tag{3.677}$$

The behavior of the Dirac spinors $v(\mathbf{p}, s_3)$ is found fom this by multiplying this equation from the right-hand side with $c\chi^*(s_3)$ [recall (3.623)]. This yields

$$v(\mathbf{p}, s_3) \xrightarrow{\Lambda} v'(\mathbf{p}', s_3) = D(\Lambda)v(\mathbf{p}, s_3) = v(\mathbf{p}')W(p', \Lambda, p)c\chi^*(s_3), \tag{3.678}$$

Now we use the fact that the 2×2 -Wigner rotation can be written as $e^{-i\alpha\cdot\sigma/2}$, which satisfies the relation (3.628), so that

$$c^{-1}W(p', \Lambda, p)c = W^*(p', \Lambda, p), \tag{3.679}$$

to rewrite on the right-hand side

$$W(p', \Lambda, p)c\chi^*(s_3) = cW^*(p', \Lambda, p)\chi^*(s_3) = c\chi^*(s_3')W^*_{s_3's_3}, \tag{3.680}$$

and we obtain the transformation law for the bispinors $v(\mathbf{p}, s_3)$:

$$v(\mathbf{p}, s_3) \xrightarrow{\Lambda} v'(\mathbf{p}', s_3) = D(\Lambda)v(\mathbf{p}, s_3) = \sum_{s_3'=-1/2}^{1/2} v(\mathbf{p}', s_3')W^*_{s_3's_3}(p', \Lambda, p), \quad (3.681)$$

Thus we find that under Lorentz transformations, the spin orientations of the bispinors $v(\mathbf{p}, s_3)$ are linearly recombined with each other by the complex-conjugate Wigner rotations $W^*_{s_3's_3}(p', \Lambda, p)$. This is a consequence of the presence of the matrix c in the 4×2 -matrices (3.609) for $v(\mathbf{p})$, which has reversed canonical spin indices.

Had we used the bispinors $v(\mathbf{p}, s_3)$ in the form (3.623), the same result would have been obtained from the observation (3.627), that the spin indices of the charge-conjugate Pauli spinors $\chi^c(s_3)$ are linearly recombined with each other by the complex-conjugate rotation matrix.

The transformation properties (3.676) and (3.677) can be verified most easily in an infinitesimal form for spinors at rest. If Λ is an infinitesimal rotation R with the 4×4 -matrix $R^\mu{}_\nu = \delta^\mu{}_\nu - i\boldsymbol{\varphi} \cdot \mathbf{L}^\mu{}_\nu$, the left-hand sides must be multiplied by $D(\Lambda) = R = 1 - i\boldsymbol{\varphi} \cdot \boldsymbol{\Sigma}/2$, where Σ^i is given by (3.468). This produces the same infinitesimal Wigner rotation on the right-hand sides $1 - i\boldsymbol{\varphi} \cdot \boldsymbol{\sigma}/2$. Thus we have the relations

$$i\Sigma^i u(\mathbf{0}) = u(\mathbf{0})i\sigma^i, \qquad i\Sigma^i v(\mathbf{0}) = v(\mathbf{0})i\sigma^i. \quad (3.682)$$

Using (3.608) and (3.609), these become explicitly

$$i\Sigma^i \begin{pmatrix} \sigma^0 \\ \sigma^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 \\ \sigma^0 \end{pmatrix} i\sigma^i, \qquad i\Sigma^i \begin{pmatrix} \sigma^0 \\ -\sigma^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma^0 \\ -\sigma^0 \end{pmatrix} c(-i\sigma^i)^*. \quad (3.683)$$

Let us also write down the Wigner rotations for the helicity spinors (3.656). Since they arise from the 4×2 -matrix solutions (3.608) by a multuplication from the right with the 2×2 rotation matrix (3.651), a Lorentz transformation of $u_h(\mathbf{p}, \lambda)$ yields obviously

$$u_h(\mathbf{p}, \lambda) \xrightarrow{\Lambda} {u_h}'(\mathbf{p}', \lambda) = D(\Lambda)u_h(\mathbf{p}, \lambda) = \sum_{\lambda'=-1/2}^{1/2} u_h(\mathbf{p}', \lambda')W_{h\,\lambda'\lambda}(p', \Lambda, p). \quad (3.684)$$

with the helicity form of the Wigner rotation

$$W_h(p', \Lambda, p) = R^{-1}(\hat{\mathbf{p}}')W(p', \Lambda, p)R(\hat{\mathbf{p}}). \quad (3.685)$$

Similarly,

$$v_h(\mathbf{p}, \lambda) \xrightarrow{\Lambda} {v_h}'(\mathbf{p}', \lambda) = D(\Lambda)v_h(\mathbf{p}, \lambda) = \sum_{\lambda'=-1/2}^{1/2} v_h(\mathbf{p}', \lambda')W^{H*}_{\lambda',\lambda}(p', \Lambda, p). \quad (3.686)$$

with

$$W^{H*}(p', \Lambda, p) = R^{-1\,*}(\hat{\mathbf{p}}')W^*(p', \Lambda, p)R^*(\hat{\mathbf{p}}). \quad (3.687)$$

3.16 THOMAS PRECESSION

The properties of relativistic spinors under Lorentz transformations are crucial for a phenomenon known in atomic physics as *Thomas precession*. Consider an electron moving around an atomic nucleus. In each time interval Δt, it receives a small centripetal Lorentz boost changing its momentum. Let us see what happens to the upper two components of the canonical bispinors $u(\mathbf{p}, s_3)$ which are explicitly

$$\xi(\mathbf{p}, s_3) = B_{\hat{\boldsymbol{\zeta}}}(\zeta)\chi(s_3) = e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}\chi(s_3). \tag{3.688}$$

At an instant of time t, the electron moves with a certain velocity through space. Its state can be described by the two-component spinor $\xi(\mathbf{p}, s_3)$ defined in Eq. (3.670). As the atomic force acts on the electron, it is accelerated towards the nucleus. Thus, after s small time interval Δt, the electron will have a new momentum and a spinor $\xi(\mathbf{p}', s_3)$ which can be obtained from the first by applying a small Lorentz transformation $D^{(\frac{1}{2},0)}(\Lambda)$ to the spinor $\xi(\mathbf{p}, s_3)$ which changes its momentum $\mathbf{p}$ to $\mathbf{p}'$. The resulting transformation is split as in (3.671): into three factors. The first is a pure boost in the $-\mathbf{p}$ direction, which brings the four-momentum p to its rest frame where it is $p_R = (M, \mathbf{0})$. The second factor is a rotation, and the third is a boost into the final four-momentum p'. In this process, the spin indices of the spinor $\xi(\mathbf{p}, s_3)$ are linearly recombined with each other by a Wigner rotation according to Eq, (3.672). Let us calculate this, taking advantage of the fact that Λ is a very small pure Lorentz transformation to be denoted by

$$D^{(\frac{1}{2},0)}(\Lambda) = e^{-\boldsymbol{\epsilon}\cdot\boldsymbol{\sigma}/2}. \tag{3.689}$$

Then $\boldsymbol{\zeta}'$ differs very little from $\boldsymbol{\zeta}$. It will be equal to $\boldsymbol{\zeta} + \Delta\boldsymbol{\zeta}$, where $\Delta\boldsymbol{\zeta}$ is a small rapidity of the order of $\boldsymbol{\epsilon}$. To indicate the smallness of the associated rotation vector $\boldsymbol{\alpha}$ in the Wigner rotation we shall rename it to $\Delta\boldsymbol{\alpha}$. Its size is calculated from

$$e^{-i\Delta\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}/2} = e^{(\boldsymbol{\zeta}+\Delta\boldsymbol{\zeta})\cdot\boldsymbol{\sigma}/2} e^{-\boldsymbol{\epsilon}\cdot\boldsymbol{\sigma}/2} e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}. \tag{3.690}$$

Before calculating $\Delta\boldsymbol{\alpha}$, let us estimate its form and sign for slowly moving particles where $\boldsymbol{\epsilon}$, $\Delta\boldsymbol{\zeta}$, and $\boldsymbol{\zeta}$ are all of the same order. Then $\Delta\boldsymbol{\zeta}$ is equal to $\boldsymbol{\epsilon}$ up to *real* terms of order $\boldsymbol{\epsilon}^2$, and we can expand both sides of (3.690) up to the second order in all quantities as follows

$$\begin{aligned} 1 - i\Delta\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}/2 \;\approx\;& \Big[1 + (\boldsymbol{\zeta} + \Delta\boldsymbol{\zeta})\cdot\boldsymbol{\sigma}/2 + (\boldsymbol{\zeta} + \Delta\boldsymbol{\zeta})^2/4\Big] \\ \times\;& \Big[1 - \Delta\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2 + (\Delta\boldsymbol{\zeta})^2/4\Big]\Big[1 - \boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2 + \boldsymbol{\zeta}^2/4\Big] \end{aligned} \tag{3.691}$$

In the product on the right-hand side, the first-order terms cancel each other. The second-order terms decompose into hermitian and antihermitian parts. Since we are interested only in $\Delta\boldsymbol{\alpha}$, we must extract the antihermitian part. Using the identity

$$\mathbf{a}\cdot\boldsymbol{\sigma}\;\mathbf{b}\cdot\boldsymbol{\sigma} = \mathbf{a}\cdot\mathbf{b} + i\,(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}, \tag{3.692}$$

we find

$$\begin{aligned}1 - i\Delta\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}/2 &\approx 1 - i\,\{[(\boldsymbol{\zeta}+\Delta\boldsymbol{\zeta})\times\Delta\boldsymbol{\zeta}] + [(\boldsymbol{\zeta}+\Delta\boldsymbol{\zeta})\times\boldsymbol{\zeta}] - [\Delta\boldsymbol{\zeta}\times\boldsymbol{\zeta}]\}\cdot\boldsymbol{\sigma}/4 \\ &\approx 1 + i\,[\Delta\boldsymbol{\zeta}\times\boldsymbol{\zeta}]\cdot\boldsymbol{\sigma}/4. \end{aligned} \tag{3.693}$$

so that we obtain the rotation vector for small $\boldsymbol{\zeta}$:

$$\Delta\boldsymbol{\alpha} \approx \frac{1}{2}\boldsymbol{\zeta}\times\Delta\boldsymbol{\zeta}. \tag{3.694}$$

The spin matrix is rotated under a Wigner rotation as follows:

$$\boldsymbol{\sigma} \to \boldsymbol{\sigma}' = W^{-1}\boldsymbol{\sigma}W. \tag{3.695}$$

With an infinitesimal $W \approx 1 - i\Delta\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}/2$ this yields

$$\Delta\boldsymbol{\sigma} = i[\Delta\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}, \boldsymbol{\sigma}] = \Delta\boldsymbol{\alpha}\times\boldsymbol{\sigma}. \tag{3.696}$$

An accelerated point particle receives a small boost $\boldsymbol{\epsilon}$ in each small time interval Δt. In this time the spin precesses at an angular velocity $\Delta\boldsymbol{\alpha}/\Delta t$. In the limit $\Delta t \to 0$, Eq. (3.694) implies an angular velocity of Wigner rotations

$$\boldsymbol{\Omega}_{\rm T} \approx \frac{1}{2}\boldsymbol{\zeta}\times\dot{\boldsymbol{\zeta}} \approx \frac{1}{2c^2}\mathbf{v}\times\dot{\mathbf{v}}, \tag{3.697}$$

which is the angular velocity of *Thomas precession*. For the spin vector in the electron's rest frame this amounts to the rate equation

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\Omega}_T\times\mathbf{S} = \frac{1}{2c^2}(\mathbf{v}\times\dot{\mathbf{v}})\times\mathbf{S}\,. \tag{3.698}$$

For finite $\boldsymbol{\zeta}$, this acquires relativistic correction factors and becomes

$$\boldsymbol{\Omega}_{\rm T} = \frac{1}{c^2}\frac{\gamma^2}{\gamma+1}\mathbf{v}\times\dot{\mathbf{v}}. \tag{3.699}$$

The derivation of this expression is somewhat tedious and will therefore be given in Appendix 3B.

The Thomas precession has observable consequences in atomic physics. In 1926, Uhlenbeck and Goudsmit noticed that the observed Zeeman splitting of atomic levels could be explained by an electron of spin $\frac{1}{2}$. Its magnetic moment is usually expressed in terms of the combination of fundamental constants which have the dimension of a magnetic moment, the *Bohr magneton* $\mu_B = e\hbar/Mc$ as

$$\boldsymbol{\mu} = g\mu_B\frac{\mathbf{S}}{\hbar}, \qquad \mu_B \equiv \frac{e\hbar}{2Mc}, \tag{3.700}$$

where $\mathbf{S}$ is the physical spin vector which has the commutation rules

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k, \tag{3.701}$$

and g is a dimensionless number called the *gyromagnetic ratio* or *Landé factor*. For a magnetic moment with this size one can calculate the spin-orbit splitting of the atomic energy levels (to be pictured and discussed further in Fig. 4.1). It is caused by the magnetic interaction energy

$$H(r)=\frac{g}{2M^2c^2}\mathbf{S}\cdot\mathbf{L}\,\frac{1}{r}\frac{dV(r)}{dr}, \tag{3.702}$$

where $V(r)$ is the atomic potential depending only on $r=|\mathbf{x}|$. To derive this $H(r)$ we note that the spin precession of the magnetic moment is given by the magnetic field in the rest frame of the electron as

$$\frac{d\mathbf{S}}{dt}=\boldsymbol{\mu}\times\mathbf{B}_{\rm el}. \tag{3.703}$$

This, on the other hand, is entirely due to the electric field in the rest frame of the atom, from which it can be found by a Lorentz transformation to the electron's velocity

$$\mathbf{B}_{\rm el}=-\gamma\frac{\mathbf{v}}{c}\times\mathbf{E},\qquad \gamma=\frac{1}{\sqrt{1-v^2/c^2}}. \tag{3.704}$$

Since an atomic electron has a velocity ratio v/c of the order of the fine-structure constant, $\alpha\sim 1/137$, we can write approximately

$$\mathbf{B}_{\rm el}\approx-\frac{\mathbf{v}}{c}\times\mathbf{E}. \tag{3.705}$$

The electric field gives the electron an acceleration

$$\dot{\mathbf{v}}=\frac{e}{M}\mathbf{E}, \tag{3.706}$$

which can also be expressed in terms of the central Coulomb potential $V(r)$ as

$$\dot{\mathbf{v}}=-\frac{\mathbf{x}}{r}\frac{1}{M}\frac{dV}{dr}. \tag{3.707}$$

Thus we can write

$$\frac{d\mathbf{S}}{dt}=-\boldsymbol{\mu}\times\left(\frac{\mathbf{v}}{c}\times\mathbf{E}\right)=-\frac{M}{ce}\,\boldsymbol{\mu}\times(\mathbf{v}\times\dot{\mathbf{v}})=-\frac{g}{2c^2}\,\mathbf{S}\times(\mathbf{v}\times\dot{\mathbf{v}}). \tag{3.708}$$

This can be written as

$$\frac{d\mathbf{S}}{dt}=\boldsymbol{\Omega}_{\rm mg}\times\mathbf{S}, \tag{3.709}$$

where $\boldsymbol{\Omega}_{\rm mg}$ is the angular velocity of spin precession caused by the magnetic field at in the rest frame of the electron:

$$\boldsymbol{\Omega}_{\rm mg}\equiv\frac{g}{2c^2}\,\mathbf{v}\times\dot{\mathbf{v}}. \tag{3.710}$$

In the rest frame of the atom where the electron is accelerated towards the center along its orbit, this result receives a relativistic correction. To lowest order in $1/c$, we must add to $\boldsymbol{\Omega}$ the angular velocity (3.697) of the Thomas precession, such that the total angular velocity of precession becomes

$$\boldsymbol{\omega} = \boldsymbol{\omega}_{\rm mg} + \boldsymbol{\omega}_{\rm T} = \frac{g-1}{2}\,\mathbf{v}\times\dot{\mathbf{v}}. \tag{3.711}$$

It is remarkable that the relativistic correction is of the same order as the original effect.

Allowing also for an external magnetic field $\mathbf{B}_{\rm ext}$ and inserting (3.707), the spin precession rate in the electron's rest frame is

$$\begin{aligned}\frac{d\mathbf{S}}{dt} &= \boldsymbol{\mu}\times\left(\mathbf{B}_{\rm ext} + \mathbf{v}\times\frac{\mathbf{x}}{r}\frac{1}{ce}\frac{dV}{dr}\right)\\ &= \boldsymbol{\mu}\times\left(\mathbf{B}_{\rm ext} - \frac{e}{Mc}\mathbf{L}\frac{dV}{dr}\right).\end{aligned} \tag{3.712}$$

This is the equation of motion which follows via Heisenberg's equation (1.241)

$$\dot{\mathbf{S}}(t) = \frac{i}{\hbar}[\mathbf{S}(t), H(t)] \tag{3.713}$$

from the interaction energy

$$\begin{aligned}H(r) &= -\boldsymbol{\mu}\cdot\left(\mathbf{B}_{\rm ext} - \frac{1}{Mce}\mathbf{L}\frac{dV}{dr}\right)\\ &= -\frac{ge}{2Mc}\mathbf{S}\cdot\mathbf{B}_{\rm ext} + \frac{g}{2M^2c^2}\mathbf{S}\cdot\mathbf{L}\frac{1}{r}\frac{dV}{dr},\end{aligned} \tag{3.714}$$

using the commutation rules (3.701). Without external magnetic field, the angular velocity of precession is

$$\boldsymbol{\Omega}_{\rm mg} = \frac{g}{2M^2c^2}\,\mathbf{L}\,\frac{1}{r}\frac{\partial V}{\partial r}. \tag{3.715}$$

This was the formula initially used to explain the experimental level splittings, and a gyromagnetic ratio $g \approx 1$ was found for the electron. It was realized by Thomas in 1927 that the accelerations of the electron change this result as in (3.711) to

$$\boldsymbol{\Omega} = \frac{g-1}{2M^2c^2}\,\mathbf{L}\,\frac{1}{r}\frac{\partial V}{\partial r}, \tag{3.716}$$

such that the experimental data implie g to be about twice as large, i.e. $g \approx 2$.

In quantum electrodynamics, the gyromagnetic ratio will receive further small corrections, as will be discussed in detail in Chapter 10.

Let us emphasize once more that the Thomas precession is a purely kinematic effect, caused entirely by the structure of the Lorentz group. Mathematically speaking, it is due to the fact that pure Lorentz transformations do not form a subgroup of the full Lorentz group. When performing pure Lorentz transformations one after another in such a way that the final frame is again at rest with respect to the initial one, the result is always a *Wigner rotation*.

3.16.1 Spin Four-Vector and Little Group

The working of the Wigner rotations in the little group found in Section 3.15 can be understood independently of the particular spinors. For any massive elementary of composite physical system we introduce a quantity called *total spin four-vector*. It is a combination of the total angular momentum $\hat{J}^{\mu\nu} = \hat{L}_{\mu\nu} + S_{\mu\nu}$ with the total momentum operator $\hat{p}$ into a vector

$$\hat{S}_\mu = \frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\hat{J}^{\nu\lambda}\hat{p}^\kappa \tag{3.717}$$

where $\epsilon_{\mu\nu\lambda\kappa}$ is the totally antisymmetric unit matrix with $\epsilon^{0123} = 1$. For massive elementary particles of momentum p^μ, the time and space components of the spin four-vector become explicitly

$$\hat{S}^0 = \mathbf{p}\cdot\hat{\mathbf{J}}, \qquad \hat{\mathbf{S}} = p^0\hat{\mathbf{J}} - \mathbf{p}\times\hat{\mathbf{K}}, \tag{3.718}$$

where $\hat{\mathbf{J}} = (\hat{J}^{23}, \hat{J}^{31}, \hat{J}^{12})$ and $\mathbf{K} = (\hat{J}^{01}, \hat{J}^{02}, \hat{J}^{03})$. Studying particles at fixed momenta, we have dropped operator hats on the momenta in (3.718), and the generators of orbital angular momentum orbital $\hat{L}_{\mu\nu}$ become differential operators in momentum space and read explicitly [compare (3.90)]

$$\hat{L}_{\mu\nu} \equiv i(p_\mu\partial_\nu - p_\nu\partial_\mu) \tag{3.719}$$

with $\partial_\mu \equiv \partial/\partial p^\mu$.

Using the commutation relations (3.272) and (3.93), the components of $\hat{S}^\mu$ in (3.717) can be shown to satisfy the commutation rules

$$[\hat{S}^\mu, \hat{S}^\nu] = i\epsilon^{\mu\nu}{}_{\lambda\kappa}\hat{S}^\lambda\hat{p}^\kappa. \tag{3.720}$$

The proof makes use of the tensor identity (3.233) which, after taking advantage of the antisymmetry of $\hat{J}^{\lambda\lambda'}$ in the indices λ and λ' and the symmetry of $p^\kappa p^{\kappa'}$ in κ and κ', leads to

$$\epsilon_{\mu\nu\lambda\kappa}\epsilon^{\mu}{}_{\lambda'\kappa'}{}^{\nu'}\hat{J}^{\lambda\lambda'}p^\kappa p^{\kappa'} = \frac{1}{2}\epsilon_{\mu\kappa}{}^{\nu\nu'}\epsilon^{\mu}{}_{\lambda\lambda'\kappa'}\hat{J}^{\lambda\lambda'}p^\kappa p^{\kappa'}, \tag{3.721}$$

and thus to the right-hand side of (3.720).

The same result can of course be derived without the lengthy identity (3.233) by considering time and space components in (3.718) separately using the commutators (3.72), (3.74), and (3.93). Then we find

$$\begin{aligned} [\hat{L}_i, p^0] &= 0, & [\hat{L}_i, p^j] &= i\epsilon_{ijk}p^k, \\ [\hat{M}_i, p^0] &= -ip^i, & [\hat{M}_i, p^j] &= -i\delta^{ij}p^0. \end{aligned} \tag{3.722}$$

For a free particle, p^μ is independent of time, and so is $\hat{S}^\mu$. By definition, the spin four-vector $\hat{S}^\mu$ is orthogonal to the four-mometum:

$$\hat{S}^\mu p_\mu = 0. \tag{3.723}$$

The physical significance of $\hat{S}^\mu$ becomes clear by going into the rest frame of a massive particle where the system has no velocity, so that [recall (3.20)]

$$p_R^\lambda = Mc(1,0,0,0). \tag{3.724}$$

Then

$$\begin{aligned} \hat{S}_R^0 &= 0 \\ \hat{S}_R^i &= Mc\frac{1}{2}\epsilon^{ijk}\hat{J}^{ik} \equiv Mc\,\hat{J}_i. \end{aligned} \tag{3.725}$$

Removing an overall factor Mc, we define the operators of Wigner rotations

$$\hat{W}^i \equiv \hat{S}_R^i/Mc, \tag{3.726}$$

satisfying he commutation relations

$$[\hat{W}^i, \hat{W}^j] = i\epsilon_{ijk}\hat{W}^k. \tag{3.727}$$

Thus the total spin four-vector has the property that its spatial components coincide in the rest frame with the total angular momentum of the system. This is certainly time independent due to angular momentum conservation.

Moreover, at zero momentum, the orbital part of $\hat{J}^i$ vanishes, so that only the spin part S^i of $\hat{J}^i$ survives, and we can drop the hats on top of S_R^i which indicate the presence of differential operators. Then we obtain pure spin matrices for the operators $\hat{W}^i$

$$W^i \equiv S_R^i/Mc, \tag{3.728}$$

satisfying the same commutation relations as the operators in (3.727). They will be called *spin three-vectors.*

The relation between the spin three-vector and the spin four-vector is obtained by applying the pure Lorentz transformation matrix (3.17) to (3.725), yielding

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}_R + \frac{\gamma^2}{\gamma+1}\frac{1}{c^2}(\hat{\mathbf{S}}_R\cdot\mathbf{v})\mathbf{v}, \quad \hat{S}^0 = \frac{1}{c}\,. \tag{3.729}$$

From (3.723) we obtain

$$\hat{S}^0 = \frac{1}{c}\,\mathbf{S}\cdot\mathbf{v}. \tag{3.730}$$

The inverse of relation (3.729) is

$$\hat{\mathbf{S}}_R = \hat{\mathbf{S}} - \frac{\gamma}{\gamma+1}\frac{1}{c^2}(\mathbf{S}\cdot\mathbf{v})\mathbf{v}, \quad \hat{S}_R^0 = 0, \tag{3.731}$$

as can be verified with the help of the relation

$$\frac{v^2}{c^2} = \frac{\gamma^2-1}{\gamma^2}, \tag{3.732}$$

which implies that $\gamma/(\gamma-1)c^2 = (\gamma-1)/\gamma v^2$. Note that

$$\mathbf{v}\cdot\mathbf{S} = \gamma\mathbf{v}\cdot\mathbf{S}_R. \tag{3.733}$$

If a point article moves in an orbit under the influence of a torque-free central force (for example, an electron around a nucleus in an atom), the total angular momentum is conserved. The spin, however, performs a Thomas precession of Section (3.16). This precession follows the covariant equation of motion

$$\frac{d\hat{S}_\mu}{d\tau} = -\frac{1}{M^2c^2}\hat{S}_\lambda\frac{dp^\lambda}{d\tau}p_\mu. \tag{3.734}$$

Note that the direction of $d\hat{S}_\mu/d\tau$ is the same as that of p^μ. Let us verify that this equation yields indeed the Thomas precession. For a slowly moving particle, it yields in the Lorentz frame of the atom

$$\frac{d\hat{\mathbf{S}}}{dt} \approx \frac{1}{M^2c^2}\left(\hat{\mathbf{S}}\cdot\frac{d\mathbf{p}}{dt}\right)\mathbf{p} \approx \frac{1}{c^2}\left(\hat{\mathbf{S}}\cdot\dot{\mathbf{v}}\right)\mathbf{v}. \tag{3.735}$$

We now use Eq. (3.731) to find the rate of precession in the rest frame of the electron which moves with $v \ll c$ through the atom

$$\frac{d\hat{\mathbf{S}}_R}{dt} \approx \frac{d}{dt}\hat{\mathbf{S}} - \frac{1}{2c^2}\left[(\hat{\mathbf{S}}\cdot\dot{\mathbf{v}})\mathbf{v} + (\hat{\mathbf{S}}\cdot\mathbf{v})\dot{\mathbf{v}}\right] \tag{3.736}$$

Inserting here (3.735) we find

$$\frac{d\hat{\mathbf{S}}_R}{dt} \approx \frac{1}{2c^2}\left[(\hat{\mathbf{S}}\cdot\dot{\mathbf{v}})\mathbf{v} - (\hat{\mathbf{S}}\cdot\mathbf{v})\dot{\mathbf{v}}\right] = -\frac{1}{2c^2}\,(\mathbf{v}\times\dot{\mathbf{v}})\times\mathbf{S}. \tag{3.737}$$

This agrees precisely with the previous rate equation (3.698) of Thomas precession. Thomas derived a general fully relativistic formula for the precession frequency of the spin of the electron in its rest frame while moving through external electric and magnetic fields which reads[20]

$$\Omega_T = -\frac{e}{Mc}\left[\left(\frac{g}{2}-1+\frac{1}{\gamma}\right)\mathbf{B} - \left(\frac{g}{2}-1\right)\frac{\gamma}{\gamma+1}\frac{1}{c^2}\left(\mathbf{v}\cdot\mathbf{B}\right)\mathbf{v} - \left(\frac{g}{2}-\frac{\gamma}{\gamma+1}\right)\frac{1}{c}\mathbf{v}\times\mathbf{B}\right]. \tag{3.738}$$

Its is equivalent to the manifestly covariant Bargmann-Michel-Telegdi equation[21]

$$\frac{dS^\mu}{d\tau} = \frac{e}{Mc}\left[\frac{g}{2}F^{\mu\nu}S_\nu + \frac{1}{M^2c^2}\left(\frac{g}{2}-1\right)\left(S_\lambda F^{\lambda\nu}p_\nu\right)p^\mu\right]. \tag{3.739}$$

For massless particles, the Wigner rotations have quite different properties than for massive particles. In the special reference frame in which the massless particle runs along the z-axis with a reference momentum $p_R^\mu = (1,0,0,1)p$ introduced in (3.24), these components become

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[20] L.T. Thomas, Phil. Mag. *3*, 1 (1927).

[21] V. Bargmann, L. Michel, and V.L. Telegdi, Phys. Rev. Lett. *2*, 435 (1959).

$$\hat{S}^0 = p\,\hat{J}^3, \quad \hat{S}^1 = p\,(J^1 + K^2), \quad \hat{S}^3 = p\,(\hat{J}^2 - \hat{K}^1), \quad \hat{S}^3 = p\,\hat{J}^3. \tag{3.740}$$

The three independent components

$$\hat{W}^3 \equiv \hat{S}^0 = \hat{S}^3, \qquad W^1 \equiv \hat{S}^1, \qquad W^2 \equiv \hat{S}^1 \tag{3.741}$$

satisfy the commutation relations

$$[\hat{W}^3, \hat{W}^1] = i\hat{W}^2, \quad [\hat{W}^3, \hat{W}^2] = -i\hat{W}^1, \quad [\hat{W}^1, \hat{W}^2] = 0. \tag{3.742}$$

These generate a *euclidean group* in a plane. Recall the definition of this group. In D diemnsions, it consists of $D(D-1)$ generators L_{ij} of the D-dimensional rotation group:

$$[L_{ij}, L_{ik}] = iL_{jk}, \tag{3.743}$$

and D genrators of translation p_i, which commute with each other and are vecotr operators under rotations:

$$[p_i, p_j] = 0, \qquad [L_{ij}, p_k] = i\left(\delta_{ik}p_j - \delta_{jk}p_i\right). \tag{3.744}$$

These commutation rules can be ontained from those of the Lorentz group in D-dimensions [see Eqs. (3.72)–(3.74)] by setting $p_i = M_i/c$ and letting c go to infinity. This construction is called *group contraction*.

The commuting generators $\hat{W}^1$ and $\hat{W}^2$ can be diagonalized simultaneously like commuting momentum operators in a plane with arbitrary continouous eigenvalues w^1 and w^2, respectively. The third generator $\hat{W}^3$ generates rotations in this plane with discrete eigenvalues $w^3 = \lambda$, where λ are azimuthal quantum numbers. which can be equal to an integer of a half-integer number. In mirror-symmetric theries, both signs have to occur. In an arbitrary reference frame, $\hat{W}^0$ is given, according to (3.718), by the operator $\hat{W}^0 = \mathbf{p}\cdot\mathbf{J}/p$. This shows that the eigenvalues λ measure the angular momentum around the momentum dierection, i.e., the helicity of the particle.

It turns out that in nature, all massless particles happen to follow a representation of the Wigner algebra which have only trivial eigenvalues $w^1 = w^2 = 0$. They are characterizes completely by the helicity, which is unchanged under Wigner rotations, but merely receives a pure phase factor which multiplies the helicity spinors or massless polarization vectors.

The occurence of only such a subset of all possible zero-mass reresentations can be understood by a limiting process such as the one performed in the derivation of the massless spinors (3.665) and (3.666). We imagine for a moment that all massless particles carry a small mass which we let go to zero. It can then be vverified that the limiting spinors change under a Lorentz transformation merely by a phase factor associated with helicity $\lambda = \pm 1/2$.:

$$\begin{aligned} D(\Lambda)u_R(\mathbf{p}) &= u_R(\mathbf{p})e^{i\omega(p',\Lambda,p)/2}, \quad & D(\Lambda)u_L(\mathbf{p}) &= u_L(\mathbf{p})e^{-i\omega(p',\Lambda,p)/2}, \\ D(\Lambda)v_R(\mathbf{p}) &= u_R(\mathbf{p})e^{-i\omega(p',\Lambda,p)/2}, \quad & D(\Lambda)u_L(\mathbf{p}) &= u_L(\mathbf{p})e^{i\omega(p',\Lambda,p)/2}. \end{aligned} \tag{3.745}$$

For the polarization vectors of electromagnetism $\epsilon^{\mu}(\mathbf{k},\lambda)$ in (3.296), and the tensors $\epsilon^{\mu\nu}(\mathbf{k},\lambda)$ of gravity in (3.383) we have, similarly:

$$\Lambda^{\mu}{}_{\nu}\epsilon^{\nu}(\mathbf{p},\lambda) = \epsilon^{\mu}(\mathbf{p},\lambda)e^{i\lambda\omega(p',\Lambda,p)}, \quad \Lambda^{\mu}{}_{\nu}\Lambda^{\mu'}{}_{\nu'}\epsilon^{\nu\nu'}(\mathbf{p},\lambda) = \epsilon^{\mu\mu'}(\mathbf{p},\lambda)e^{i\lambda\omega(p',\Lambda,p)}. \tag{3.746}$$

The reader is invited to derive this directly from the explicit expressions for these objects.

3.17 WEYL'S SPINOR CALCULUS

Weyl has devised a simple calculus for constructing spinor invariants of the Lorentz group. It is very similar to the tensor calculus. The spinor in the upper two components of the Dirac field, which transforms under boosts via the matrix $e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}$, was previously denoted by ξ_{α}, the spinor in the lower component, transforming via $e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}$, by $\eta^{\dot{\beta}}$. Complex conjugation brings ξ_{α} into a spinor $(\xi_{\alpha})^*$ which transforms via $e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}^*/2}$. Such a spinor is given a lower dotted index, i.e., we write

$$(\xi_{\alpha})^* \equiv \xi^*{}_{\dot{\alpha}}. \tag{3.747}$$

Similarly, we define $(\eta^{\dot{\beta}})^*$ which transforms via $e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}^*/2}$ as

$$(\eta^{\dot{\beta}})^* \equiv \eta^{*\beta}. \tag{3.748}$$

From the earlier discussion in Section 3.12 we know that

$$(\eta^{\dot{\alpha}})^*\xi_{\alpha}, \quad (\xi_{\beta})^*\eta^{\dot{\beta}} \tag{3.749}$$

are Lorentz invariants. With the above notation, these can be viewed as

$$\eta^{*\alpha}\xi_{\alpha}, \quad \xi^*{}_{\dot{\beta}}\eta^{\dot{\beta}}. \tag{3.750}$$

Thus the invariants arise by simple contractions of equal upper and lower indices.

A further invariant can be constructed from two spinors which both have lower indices α and β, namely

$$\xi'_{\beta}\, c^{\beta\alpha}\, \xi_{\alpha}, \tag{3.751}$$

with the 2×2 -charge conjugation matrix $c = -i\sigma^2$ of (3.543). Writing (3.751) in matrix notation as $\xi'^{T}c\xi$, it goes under rotations over into

$$\xi'^{T}e^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}^{T}/2}ce^{-i\boldsymbol{\varphi}\cdot\boldsymbol{\sigma}/2}\xi. \tag{3.752}$$

Since $\boldsymbol{\sigma}^T = \boldsymbol{\sigma}^*$ [see (3.400)] and $\boldsymbol{\sigma}^* c = -c\boldsymbol{\sigma}$ from (3.578), this is obviously invariant. A similar manipulation shows invariance under boosts. Thus the matrix $c^{\alpha\beta}$ constitutes an antisymmetric (or symplectic) metric in spinor space. Accordingly, we define

$$\xi^\beta \equiv c^{\beta\alpha}\xi_\alpha. \tag{3.753}$$

Then the invariant (3.751) arises by a contraction of equal upper and lower indices, just as in the notation in Minkowski space:

$$\xi'_\beta c^{\beta\alpha}\xi_\alpha = \xi'^\alpha \xi_\alpha. \tag{3.754}$$

Similarly, we can form an invariant from two $\eta^{\dot\beta}$-spinors

$$\eta'^{\dot\beta}(c^{-1})_{\dot\beta\dot\alpha}\eta^{\dot\alpha}, \tag{3.755}$$

defining

$$\eta_{\dot\beta} \equiv (c^{-1})_{\dot\beta\dot\alpha}\eta^{\dot\alpha}, \tag{3.756}$$

which makes the contraction $\eta'_{\dot\beta}\eta^{\dot\beta}$ a Lorentz invariant.

The Lorentz transformation matrices associated with ξ_α and $\eta^{\dot\beta}$ are $D^{(\frac{1}{2},0)}(\Lambda)$ and $D^{(0,\frac{1}{2})}(\Lambda)$, respectively. They carry Weyl indices $D^{(\frac{1}{2},0)}(\Lambda)_\alpha{}^{\alpha'}$ and $D^{(0,\frac{1}{2})}(\Lambda)^{\dot\beta}{}_{\dot\beta'}$.

It is possible to combine Weyl spinors to vectors rather than scalars with the help of the σ^μ-matrices (3.418) and of $\tilde\sigma^\mu$. They may be thought of as carrying Weyl labels

$$(\sigma^\mu)_{\alpha\dot\beta}, \tag{3.757}$$

and

$$(\tilde\sigma^\mu)^{\dot\beta\alpha}. \tag{3.758}$$

Then the indices show directly which spinors are required to form vectors:

$$\xi^*\tilde\sigma^\mu\xi = \xi^*{}_{\dot\beta}(\tilde\sigma^\mu)^{\dot\beta\alpha}\xi_\alpha, \qquad \eta^*\sigma^\mu\eta = \eta^{*\alpha}(\sigma^\mu)_{\alpha\dot\beta}\eta^{\dot\beta}. \tag{3.759}$$

The vector nature of these combinations is proved by rewriting the transformation law (3.462) out in 2 × 2 -form:

$$\begin{aligned} D^{(\frac{1}{2},0)}(\Lambda)^{-1}\sigma^\mu D^{(0,\frac{1}{2})}(\Lambda) &= \Lambda^\mu{}_\nu\sigma^\nu, \\ D^{(0,\frac{1}{2})}(\Lambda)^{-1}\tilde\sigma^\mu D^{(\frac{1}{2},0)}(\Lambda) &= \Lambda^\mu{}_\nu\tilde\sigma^\nu. \end{aligned} \tag{3.760}$$

Written with Weyl indices, this reads

$$\begin{aligned} [D^{(\frac{1}{2},0)}(\Lambda)^{-1}]'_\beta{}^\alpha(\sigma^\mu)_{\alpha\dot\beta}D^{(0,\frac{1}{2})}(\Lambda)^{\dot\beta}{}_{\dot\beta'} &= (\sigma^\mu)_{\beta\dot\beta'}, \\ [D^{(0,\frac{1}{2})}(\Lambda)^{-1}]^{\dot\alpha}{}_{\dot\alpha'}(\tilde\sigma^\mu)^{\dot\alpha'\beta}D^{(\frac{1}{2},0)}(\Lambda)_\beta{}^{\beta'} &= (\tilde\sigma^\mu)^{\dot\alpha\beta'}. \end{aligned} \tag{3.761}$$

In Weyl's calculus, the Dirac equation reads

$$(i\partial\!\!\!/ - M)\psi(x) = \begin{pmatrix} -M\delta_\alpha{}^{\alpha'} & (i\sigma^\mu\partial_\mu)_{\alpha\dot\beta'} \\ (i\tilde\sigma^\mu\partial_\mu)^{\dot\beta\alpha'} & -M\delta^{\dot\beta}{}_{\dot\beta'} \end{pmatrix}\begin{pmatrix} \xi_{\alpha'} \\ \eta^{\dot\beta'} \end{pmatrix} = 0. \tag{3.762}$$

3.18 HIGHER-SPIN REPRESENTATIONS

Given the fundamental spin-1/2 field it is very simple to generalize the transformation matrices to higher spins. A system with two spin-1/2 particles can have spin 1 or 0. Similarly, n spin-1/2 particles can couple to spin $n/2, n-1/2, \dots$ down to 1/2 or 0. Thus in order to build an arbitrary spin s, all we have to do is put $2s$ spin-1/2 representations together in an appropriate fashion. The problem is completely analogous to the previous extension in Section 2.5 of the one-particle Schrödinger equation to an arbitrary $n-$particle equation. Thus we shall construct representations of arbitrary spin by a "second quantization" of spin, and further of the generators of the entire Lorentz group.

3.18.1 Rotations

If the particle is at rest, spin is defined by the rotation subgroup. The 2×2 hermitian generators

$$\mathbf{L}=\frac{1}{2}\boldsymbol{\sigma} \tag{3.763}$$

may be considered as the analog of the single-particle Schrödinger operator $-\frac{\hbar^2}{2M}\partial_{\mathbf{x}}{}^2+V_1(\mathbf{x};t)$ in Eq. (2.90), or as the matrix M_i in the commutation rules (2.97). According to (2.99), the second quantized version of $\mathbf{L}$ reads

$$\hat{L}_i=\frac{1}{2}\hat{a}^\dagger\,\sigma^i\,\hat{a}. \tag{3.764}$$

where $\hat{a}^\dagger_\alpha$ and $\hat{a}_\alpha$ with $\alpha=1,2$ are two bosonic creation and annihilation operators. As proved in general in (2.100), these operators satisfy the same commutation rules as the Pauli matrices σ^i:

$$[\hat{L}_i,\hat{L}_j]=i\epsilon_{ijk}\hat{L}_k. \tag{3.765}$$

The states

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle\equiv\hat{a}^\dagger_1|0\rangle,\qquad |\tfrac{1}{2},-\tfrac{1}{2}\rangle\equiv\hat{a}^\dagger_2|0\rangle \tag{3.766}$$

may be identified as the two basis states of the fundamental spin-1/2 representation. The effect of the three operators $\hat{L}_i$ is, as in the general Eq. (2.101):

$$\begin{aligned}\left[\hat{L}_i,\hat{a}^\dagger_\alpha\right] &= \hat{a}^\dagger_{\alpha'}\frac{1}{2}\sigma^i_{\alpha'\alpha},\\ \left[\hat{a}_{\alpha'},\hat{L}_i\right] &= \frac{1}{2}\sigma^i_{\alpha'\alpha}\hat{a}_\alpha.\end{aligned} \tag{3.767}$$

On these states, the second-quantized operators (3.764) have eigenvalues

$$\hat{\mathbf{L}}|s,s_3\rangle=s(s+1)|s,s_3\rangle,\qquad \hat{L}_3|s,s_3\rangle=s_3|s,s_3\rangle. \tag{3.768}$$

In the present restriction to the rotation group we shall use only lower indices 1 and 2 rather than Weyl indices of the previous section.

As in Section 2.5, we may now compose all higher representations of the rotation group by combining many of these fundamental representations, and forming states such as

$$\prod_{i=1}^{2s}(a^{\dagger}_{\alpha_i})|0\rangle. \tag{3.769}$$

It is easy to see that linear combinations of such states with a fixed number of $a^{\dagger}$ form an invariant representation space of the rotation group. The reason is that the three generators $\hat{L}_i$ commute with the "particle" number operator

$$N = \hat{a}^{\dagger}\hat{a}. \tag{3.770}$$

In fact, a little algebra shows that the *Casimir operator* of the rotation group $\hat{\mathbf{L}}^2$ which characterizes an irreducible representation is equal to

$$\hat{\mathbf{L}}^2 = \frac{1}{4}(\hat{a}^{\dagger}\,\sigma^i\,\hat{a})^2 = \frac{1}{2}\hat{N}\left(\frac{1}{2}\hat{N}+1\right), \tag{3.771}$$

showing explicitly that under rotations, states built from a fixed number $2s$ of spin creation operators $a^{\dagger}$ always maintains the same number $2s$, and that the eigenvalue of the Casimir operator in the space of $2s$ particles is $s(s+1)$. Thus the space is indeed *invariant* under rotations.

But it is also an irreducible representation of spin s. To see this take the complete set of basis states in the space

$$|n_1, n_2) = \frac{1}{\sqrt{n_1!n_2!}}(\hat{a}^{\dagger}_1)^{n_1}(\hat{a}^{\dagger}_2)^{n_2}|0\rangle, \tag{3.772}$$

which diagonalize the occupation numbers of the two operators $a^{\dagger}_1$ and $a^{\dagger}_2$, and which are normalized to unity. Applying to these the operator

$$\hat{L}_3 = \hat{a}^{\dagger}\frac{\sigma^3}{2}\hat{a} = \frac{1}{2}(\hat{a}^{\dagger}_1\hat{a}_1 - a^{\dagger}_2 a_2), \tag{3.773}$$

we see that it measures the difference in the number of "spin up" and "spin down" particles created by $a^{\dagger}_1$ and $a^{\dagger}_1$, respectively:

$$L_3|n_1, n_2) = \frac{1}{2}(n_1 - n_2)|n_1, n_2) \equiv m|n_1, n_2). \tag{3.774}$$

Thus the state has the azimuthal ("magnetic") quantum number $m = n_1 - n_2$. The operators

$$\hat{L}_+ \equiv \hat{L}_1 + i\hat{L}_2, \quad \hat{L}_- \equiv \hat{L}_1 - i\hat{L}_2, \tag{3.775}$$

on the other hand, have the form

$$\begin{aligned} \hat{L}_+ &= \hat{a}^{\dagger}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\hat{a} = \hat{a}^{\dagger}_1\,\hat{a}_2 \\ \hat{L}_- &= \hat{a}^{\dagger}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\hat{a} = \hat{a}^{\dagger}_2\,\hat{a}_1. \end{aligned} \tag{3.776}$$

Among each other and with $\hat{L}_3$ they satisfy the commutation rules

$$\begin{aligned}[\hat{L}_-, \hat{L}_+] &= 2\hat{L}_3 \\ [\hat{L}_3, \hat{L}_+] &= \hat{L}_+ \\ [\hat{L}_3, \hat{L}_-] &= -\hat{L}_-. \end{aligned} \tag{3.777}$$

They remove a spin down while adding a spin up and vice versa. Their matrix elements are

$$\begin{aligned}\hat{L}_+|n_1, n_2) &= \sqrt{(n_1+1)n_2}|n_1+1,\, n_2-1), \\ \hat{L}_-|n_1, n_2) &= \sqrt{n_1(n_2+1)}|n_1-1,\, n_2+1). \end{aligned} \tag{3.778}$$

It is now obvious that starting from an arbitrary state, say $|n,\, 0)$ with no number of spin-down particles and eigenvalue $n/2$ of $\hat{L}_3$, we can reach every other state $|n-k,\, k)$ with $k = 1, \dots, n$ by repeated application of $\hat{L}_-$. The process ends at $|0,\, n)$, where $\hat{L}_-|n, 0) = 0$. This proves the irreducibility of the representation.

Conventionally, the highest eigenvalue of $\hat{L}_3$ is referred to as the value s of angular momentum:

$$s = n/2. \tag{3.779}$$

It appears in the eigenvalue (3.771) of $\hat{\mathbf{L}}^2$ as

$$\hat{\mathbf{L}}^2|n-k,\, k) = s(s+1)|n-k,\, k). \tag{3.780}$$

Hence the states may be reexpressed in terms of the numbers s and m as

$$|s, m\rangle = |s+m, s-m) = \frac{1}{\sqrt{(s-m)!(s+m)!}}(\hat{a}_1^\dagger)^{s+m}(\hat{a}_2^\dagger)^{s-m}|0\rangle, \tag{3.781}$$

and the matrix elements (3.774) and (3.778) read

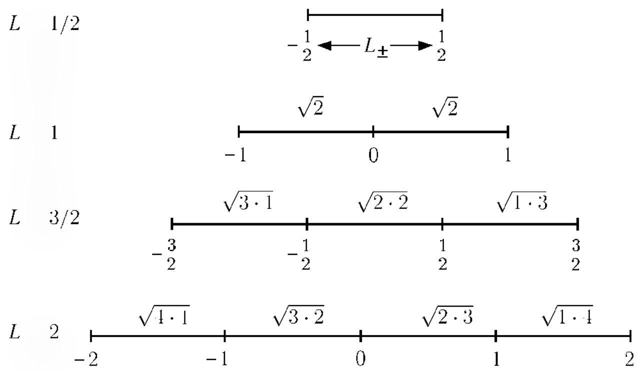
L 1/2
1
$-\frac{1}{2}$ $L_\pm$ $\frac{1}{2}$
L 1
$\sqrt{2}$ $\sqrt{2}$
−1 0 1
L 3/2
$\sqrt{3\cdot 1}$ $\sqrt{2\cdot 2}$ $\sqrt{1\cdot 3}$
$-\frac{3}{2}$ $-\frac{1}{2}$ $\frac{1}{2}$ $\frac{3}{2}$
L 2
$\sqrt{1\cdot 1}$ $\sqrt{3\cdot 2}$ $\sqrt{2\cdot 3}$ $\sqrt{1\cdot 4}$
−2 −1 0 1 2

FIGURE 3.3 Effect of raising and lowering operators $\hat{L}_+$ and $\hat{L}_-$ upon the states $|s, m\rangle$.

$$\hat{L}_3|s, m\rangle = m|s, m\rangle, \tag{3.782}$$

$$\hat{L}_+|s, m\rangle = \sqrt{(s-m)(s+m+1)}|s, m+1\rangle, \tag{3.783}$$

$$\hat{L}_-|s, m\rangle = \sqrt{(s+m)(s-m+1)}|s, m-1\rangle. \tag{3.784}$$

For smaller spin values the effect of the raising and lowering operators $\hat{L}_+$ and $\hat{L}_-$ upon the states $|s,m\rangle$ is illustrated in Fig. 3.3.

Note that we could have defined the states (3.781) with arbitrary phase factors $e^{i\phi_1}$ and $e^{i\phi_2}$ accompanying $a_1^\dagger$ and $a_2^\dagger$. Then the application of L_+ and L_- would produce phase factors $e^{-i(\phi_1-\phi_2)}$ and $e^{i(\phi_1-\phi_2)}$ in (3.783) and (3.784), respectively. It is easy to verify that these phases drop out in the commutation rules (3.777) of the rotation group, and thus in (3.765).

The choice of a positive-square root in (3.783) and (3.784) without such extra phase factors is known as the *Condon-Shortley phase convention.*[22]

3.18.2 Extension to Lorentz Group

It is now quite simple to extend this construction of spin representations of the rotations to the entire Lorentz group. For this we deduce from the commutation rules between the generators L_i and M_i in Eq. (3.72) (3.74) that the combinations

$$\begin{aligned}\hat{\mathbf{J}}^1 &= (\hat{\mathbf{L}}+i\hat{\mathbf{M}})/2,\\ \hat{\mathbf{J}}^2 &= (\hat{\mathbf{L}}-i\hat{\mathbf{M}})/2\end{aligned}\tag{3.785}$$

have the commutation rules

$$\begin{aligned}\left[\hat{J}_i^1,\hat{J}_j^2\right] &= 0,\\ \left[\hat{J}_i^1,\hat{J}_j^1\right] &= i\epsilon_{ijk}\hat{J}_k^1,\\ \left[\hat{J}_i^2,\hat{J}_j^2\right] &= i\epsilon_{ijk}\hat{J}_k^2.\end{aligned}\tag{3.786}$$

Therefore they generate two independent sets of rotations. Extending the previous construction, we now form the second-quantized operators

$$\begin{aligned}\hat{\mathbf{J}}^{(1)} &= \hat{a}^\dagger\frac{\boldsymbol{\sigma}}{2}\hat{a},\\ \hat{\mathbf{J}}^{(2)} &= \hat{b}^\dagger\frac{\boldsymbol{\sigma}}{2}\hat{b},\end{aligned}\tag{3.787}$$

and obtain

$$\hat{\mathbf{L}} = \hat{\mathbf{J}}^{(1)}+\hat{\mathbf{J}}^{(2)} = \hat{a}^\dagger\frac{\boldsymbol{\sigma}}{2}\hat{a}+\hat{b}^\dagger\frac{\boldsymbol{\sigma}}{2}\hat{b},\tag{3.788}$$

$$\hat{\mathbf{M}} = \frac{1}{i}(\hat{\mathbf{J}}^{(1)}-\hat{\mathbf{J}}^{(2)}) = \frac{1}{i}\left(\hat{a}^\dagger\frac{\boldsymbol{\sigma}}{2}\hat{a}-\hat{b}^\dagger\frac{\boldsymbol{\sigma}}{2}\hat{b}\right).\tag{3.789}$$

These operators correspond to forming the second-quantized operators

$$\hat{\mathbf{L}} = \frac{1}{2}(\hat{a}^\dagger,\hat{b}^\dagger)\,\boldsymbol{\Sigma}\begin{pmatrix}\hat{a}\\ \hat{b}\end{pmatrix},\tag{3.790}$$

$$\hat{\mathbf{M}} = \frac{1}{2}(\hat{a}^\dagger,\hat{b}^\dagger)\,i\boldsymbol{\alpha}\begin{pmatrix}\hat{a}\\ \hat{b}\end{pmatrix},\tag{3.791}$$

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[22] E.U. Condon and G.H. Shortley, *Theory of Atomic Spectra*, Cambridge University Press, New York, 1935.

with the 4×4 -representation matrices (3.468) and (3.470) of the Lorentz group.

For a clearer display of the Lorentz transformation properties one may take advantage of the Weyl notation. From (3.788) and (3.789) we see that the operators $a^\dagger$ and $b^\dagger$ transform according to the fundamental representations $D^{(\frac{1}{2},0)}$ and $D^{(0,\frac{1}{2})}$, since the 2×2 -matrices between them are for rotations $\boldsymbol{\sigma}/2$, $-i\boldsymbol{\sigma}/2$ and for Lorentz boosts $\boldsymbol{\sigma}/2$, $i\boldsymbol{\sigma}/2$,respectively. Thus we may write them in the Weyl notation as $a^\dagger_\alpha$ and $b^{\dagger\,\dot\beta}$. By applying the same arguments as for the rotation group to the operators $\hat{\mathbf{J}}^{(1)}$ and $\hat{\mathbf{J}}^{(2)}$, we can now easily see that the set of states

$$|n_1^a, n_2^a, n_1^b, n_2^b\rangle = \frac{1}{\sqrt{n_1^a! n_2^a! n_1^b! n_2^b!}}(\hat{a}_1^\dagger)^{n_1^a}(\hat{a}_2^\dagger)^{n_2^a}(\hat{b}^{\dagger\,\dot{1}})^{n_1^b}(\hat{b}^{\dagger\,\dot{2}})^{n_2^b}|0\rangle \tag{3.792}$$

for fixed numbers $n^a = n_1^a + n_2^a$ and $n^b = n_1^b + n_1^b$ are irreducible representation spaces of the whole Lorentz group. They are denoted by

$$(s_1, s_2) \equiv \left(\frac{n^a}{2}, \frac{n^b}{2}\right). \tag{3.793}$$

The states (3.792) live in the direct-product space of the two operators $\hat{\mathbf{J}}^{(1)}$ and $\hat{\mathbf{J}}^{(2)}$. They may be relabeled by the quantum numbers of the two rotation subgroups as in (3.781):

$$\begin{aligned}|s_1, m_1; s_2, m_2\rangle = {} & \frac{1}{\sqrt{(s_1 - m_1)!(s_1 + m_1)!(s_2 - m_2)!(s_2 + m_2)!}} \\ & \times(\hat{a}_1^\dagger)^{s_1+m_1}(\hat{a}_2^\dagger)^{ns_1-m_1}(\hat{b}^{\dagger\,\dot{1}})^{s_2+m_2}(\hat{b}^{\dagger\,\dot{2}})^{s_2-m_2}|0\rangle.\end{aligned} \tag{3.794}$$

Since by (3.788) the operator of angular momentum $\hat{\mathbf{L}}$ is the direct sum of those of the two rotation subgroups, an irreducible representation $D^{(s_1,s_2)}(\Lambda)$ of the Lorentz group contains different irreducible representations of the rotation subgroup generated by $\hat{\mathbf{L}}$. They are obtained from the rules of addition of angular momenta. The operator $\hat{\mathbf{L}}^2$ and the third component $\hat{L}_3$ can be diagonalized with eigenvalues $s(s+1)$ and m by forming linear combination

$$|s, m\rangle = \sum_{m_1,m_2} |s_1, m_1; s_2, m_2\rangle\langle s_1, m_1; s_2, m_2|s, m\rangle \tag{3.795}$$

where $\langle s_1, m_1; s_2, m_2|s, m\rangle$ are *Clebsch-Gordan coefficients*. Their calculation and properties are recalled in Appendix 3C. The values of total angular momentum s occurring in the decomposition (3.795) are

$$|s_1 - s_2| \leq s \leq s_1 + s_2. \tag{3.796}$$

The Clebsch-Gordan coefficients are orthogonal and complete, so that (3.795) can be inverted to

$$|s_1, m_1; s_2, m_2\rangle = \sum_{s,m} |s, m\rangle\langle s, m|s_1, m_1; s_2, m_2\rangle. \tag{3.797}$$

3.18.3 Finite Representation Matrices

To complete this discussion let us calculate the finite representation matrices. Due to the decompositions (3.788) and (3.789), we only need those of the rotation group. This is done as follows.

Rotation Group

We first observe that every 3×3 -rotation matrix $R_{\hat{\varphi}}(\varphi)$ in Eq. (3.9) can be decomposed into Euler angles

$$R_{\hat{\varphi}}(\varphi)=e^{-i\boldsymbol{\varphi}\cdot\mathbf{L}}=e^{-i\alpha L_3}e^{-i\beta L_2}e^{-i\gamma L_3}\equiv R(\alpha,\beta,\gamma), \tag{3.798}$$

and so can the general rotation operator

$$e^{-i\boldsymbol{\varphi}\cdot\hat{\mathbf{L}}}=e^{-i\alpha\hat{L}_3}e^{-i\beta\hat{L}_2}e^{-i\gamma\hat{L}_3}\equiv\hat{R}(\alpha,\beta,\gamma). \tag{3.799}$$

Since $\hat{L}_3$ is diagonal on the states $|jm\rangle$, the finite rotation $e^{-i\boldsymbol{\varphi}\cdot\hat{\mathbf{L}}}$ acts on the states $|jm\rangle$ as

$$\begin{aligned}\hat{R}(\alpha,\beta,\gamma)|jm\rangle &= \sum_{m'=-j}^{j}|jm'\rangle e^{-i(m'\alpha+m\gamma)}\langle jm'|e^{-i\beta\hat{L}_2}|jm\rangle\\ &\equiv \sum_{m'=-j}^{j}|jm'\rangle D^j_{m',m}(\alpha,\beta,\gamma),\end{aligned} \tag{3.800}$$

so that the only nontrivial matrix elements are

$$d^j_{m'm}(\beta)=\langle jm'|e^{-i\beta\hat{L}_2}|jm\rangle. \tag{3.801}$$

For a single creation operator $\hat{a}^\dagger$, we have from (3.767):

$$\begin{aligned}[\hat{L}_2,\hat{a}_1^\dagger] &= \frac{1}{2i}[\hat{a}_1^\dagger\hat{a}_2-\hat{a}_2^\dagger\hat{a}_1,\hat{a}_1^\dagger]=\frac{i}{2}\hat{a}_2^\dagger,\\ [\hat{L}_2,\hat{a}_2^\dagger] &= \frac{1}{2i}[\hat{a}_1^\dagger\hat{a}_2-\hat{a}_2^\dagger\hat{a}_1,\hat{a}_2^\dagger]=-\frac{i}{2}\hat{a}_1^\dagger,\end{aligned} \tag{3.802}$$

and therefore

$$\begin{aligned}e^{-i\beta\hat{L}_2}\hat{a}_1^\dagger e^{i\beta\hat{L}_2} &= \hat{a}_1^\dagger\cos\frac{\beta}{2}+\hat{a}_2^\dagger\sin\frac{\beta}{2},\\ e^{-i\beta\hat{L}_2}\hat{a}_2^\dagger e^{i\beta\hat{L}_2} &= -\hat{a}_1^\dagger\sin\frac{\beta}{2}+\hat{a}_2^\dagger\cos\frac{\beta}{2}.\end{aligned} \tag{3.803}$$

Of course, this is just the statement that $\hat{a}_\alpha^\dagger|0\rangle$ transforms according to the spin-1/2-representation of the rotation group [recall (3.411)]

$$\begin{aligned}e^{-i\beta\hat{L}_2}a_\alpha^\dagger e^{i\beta\hat{L}_2} &= \hat{a}_{\alpha'}^\dagger\begin{pmatrix}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2}\end{pmatrix}^{\alpha'}{}_{\alpha}\\ &= \hat{a}_{\alpha'}^\dagger\left(e^{-i\beta\sigma^2/2}\right)^{\alpha'}{}_{\alpha}.\end{aligned} \tag{3.804}$$

But then an arbitrary state (3.781) goes over into

$$\begin{aligned} e^{-\beta L_2}|jm\rangle = & \frac{1}{\sqrt{(j-m)!(j+m)!}} \\ & \times\left(\hat{a}_1^\dagger\cos\frac{\beta}{2}+\hat{a}_2^\dagger\sin\frac{\beta}{2}\right)^{j+m}\left(-\hat{a}_1^\dagger\sin\frac{\beta}{2}+\hat{a}_2^\dagger\cos\frac{\beta}{2}\right)^{j-m}|0\rangle. \end{aligned} \tag{3.805}$$

We now expand each factor in a binomial series, reorder it, and write

$$\sum_{m'}\frac{1}{\sqrt{(j-m')!(j+m')!}}(\hat{a}_1^\dagger)^{j+m'}(\hat{a}_2^\dagger)^{j-m'}|0\rangle d^j_{m'm}(\beta), \tag{3.806}$$

with

$$\begin{aligned} d^j_{m'm}(\beta) \;=\; & \sqrt{\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}}\sum_{k=0}^{\infty}\begin{pmatrix} j+m \\ j-m'-k\end{pmatrix}\begin{pmatrix} j-m \\ k\end{pmatrix} \\ & \times(-1)^{j-m-k}\left(\cos\frac{\beta}{2}\right)^{2k+m'+m}\left(\sin\frac{\beta}{2}\right)^{2j-2k-m'-m}. \end{aligned} \tag{3.807}$$

The sum can be expressed in terms of hypergeometric functions

$$F(a,b,c;z)\equiv 1+\frac{ab}{c}z+\frac{a(a+1)\,b(b+1)}{c(c+1)}\frac{z^2}{2!}+\dots \tag{3.808}$$

as

$$\begin{aligned} d^j_{m'm}(\beta) \;=\; & \frac{(-1)^{m'-m}}{(m'-m)!}\sqrt{\frac{(j-m)!(j+m')!}{(j+m)!(j-m')!}}\left(\cos\frac{\beta}{2}\right)^{m'+m}\left(\sin\frac{\beta}{2}\right)^{m-m} \\ & \times F\left(-j+m',j+m'+1;m'-m+1;\sin^2\frac{\beta}{2}\right). \end{aligned} \tag{3.809}$$

This formula is best used only for $m' \geq m$ where the hypergeometric function is regular at the origin. For $m' < m$ one may simply use the property

$$d^j_{m'm}(\beta)=(-1)^{m'-m}d^j_{mm'}(\beta)=(-1)^{m'-m}d^j_{-m'-m}(\beta). \tag{3.810}$$

Additional useful relations are

$$d^j_{m'm}(\beta-\pi)=(-1)^{j-m'}d^j_{-m'\,m}(\beta) \tag{3.811}$$

and

$$d^j_{m'm}(\pi)=(-1)^{j+m'}\delta_{m',-m}. \tag{3.812}$$

The hypergeometric functions can also be expressed as a function of Jacobi polynomials

$$\begin{aligned} & F\left(-j+m',j+m'+1;m'-m+1;\sin^2\frac{\beta}{2}\right) \\ & \qquad =\frac{(j-m')!}{(j-m)!}(m'-m)!P_{j-m'}^{(m'-m,m'+m)}(\cos\beta). \end{aligned} \tag{3.813}$$

The matrix elements $d^l_{00}(\beta)$ coincide with the Legendre polynomials,

$$d^l_{00}(\beta) = P_l(\cos\beta), \tag{3.814}$$

and the matrix elements $d^l_{m0}(\beta)e^{i\gamma}$ are proportional to the spherical harmonics $Y_{lm}(\beta,\gamma)$:

$$d^l_{m0}(\beta)e^{i\gamma} = (-1)^m d^l_{0m}(\beta)e^{i\gamma} = \sqrt{\frac{4\pi}{2l+1}}Y_{lm}(\beta,\gamma). \tag{3.815}$$

For $j=\frac{1}{2}$ we reobtain the spinor representation of the rotation group

$$d^{1/2}_{m'm}(\beta) = \begin{pmatrix} \cos\beta/2 & -\sin\beta/2 \\ \sin\beta/2 & \cos\beta/2 \end{pmatrix} = e^{-i\beta\sigma^2/2}, \tag{3.816}$$

while for $j=1$ we find the next larger vector representation

$$d^1_{m'm}(\beta) = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\sin\beta/\sqrt{2} & \frac{1}{2}(1-\cos\beta) \\ \sin\beta/\sqrt{2} & \cos\beta & -\sin\beta/\sqrt{2} \\ \frac{1}{2}(1-\cos\beta) & \sin\beta/\sqrt{2} & \frac{1}{2}(1+\cos\beta) \end{pmatrix} \tag{3.817}$$

The indices have the order $+1/2, -1/2$ and $+1, 0, -1$, respectively.

The representation functions (3.800) of all rotations

$$D^j_{m,m'}(\alpha,\beta,\gamma) = e^{-i(m\alpha+m'\gamma)}d^j_{m,m'}(\beta) \tag{3.818}$$

have the following orthonormality properties:

$$\frac{2j+1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \int_0^{2\pi} d\gamma\, D^{j_1}_{m_1,m_1'}(\alpha,\beta,\gamma)D^{j_2}_{m_2,m_2'}(\alpha,\beta,\gamma) = \delta_{j_1,j_2}\delta_{m_1,m_2}\delta_{m_1',m_2'}. \tag{3.819}$$

At fixed m_1', m_2', one has relations

$$\frac{2j+1}{4\pi}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta\, D^{j_1}_{m_1,m_1'}(\alpha,\beta,0)D^{j_2}_{m_2,m_2'}(\alpha,\beta,0) = \delta_{j_1,j_2}\delta_{m_1,m_2}. \tag{3.820}$$

The representation matrices $D^j_{m,m'}(\alpha,\beta,\gamma)$ with $j=1$ are related to the original 3×3 -rotations $R(\alpha,\beta,\gamma)$ of Eq. (3.798) as by a similarity transformation. It is the same transformation which relates the three spherical components $\boldsymbol{\varepsilon}(\lambda)$ in Eq. (3.298) to the unit vectors (3.302). The eigenvectors (3.298) supply us with the matrix elements of the desired similarity transformation. Setting

$$\langle i|1,m\rangle \equiv \epsilon^i(m), \tag{3.821}$$

we can write, using the 3×3 matrices (3.50),

$$\begin{aligned} (L_3)_{jk} &= \sum_{m=-1}^{1}\langle j|1,m\rangle m\langle 1,m|k\rangle, \\ (L_\pm)_{jk} &= \langle j|1,\pm1\rangle\sqrt{2}\langle 1,0|k\rangle + \langle j|1,0\rangle\sqrt{2}\langle 1,\mp1|k\rangle. \end{aligned} \tag{3.822}$$

In Dirac bracket notation, the original 3 × 3-matrices $R(\alpha,\beta,\gamma)$ in (3.798) may be considered as matrix elements of the general rotation operator $\hat{R}(\alpha,\beta,\gamma)$ in (3.799) between the basis states $|i\rangle$:

$$R_{ij}(\alpha,\beta,\gamma)=\langle i|\hat{R}(\alpha,\beta,\gamma)|j\rangle. \tag{3.823}$$

From the manipulation rules of Dirac brackets it is then obvious that the matrix elements transform under finite rotations as

$$\begin{aligned}\sum_{j=1}^{3}R_{ij}\,\langle j|1,m\rangle &= \sum_{j=1}^{3}\langle i|\hat{R}(\alpha,\beta,\gamma)|j\rangle\langle j|1,m\rangle\\ &= \sum_{j=1}^{3}\sum_{m'=-1}^{1}\langle i|1,m'\rangle\langle 1,m'|\hat{R}(\alpha,\beta,\gamma)|j\rangle\langle j|1,m\rangle\\ &= \sum_{m'=-1}^{1}\langle i|1,m'\rangle\langle 1,m'|\hat{R}(\alpha,\beta,\gamma)|1,m\rangle=\sum_{m'=-1}^{1}\langle i|1,m'\rangle D^{1}_{m',m}(R),\end{aligned} \tag{3.824}$$

which may also be written in materix form as as[23]

$$R\boldsymbol{\epsilon}(m)=\sum_{m'=-1}^{1}\boldsymbol{\epsilon}(m')D^{1}_{m',m}(R). \tag{3.825}$$

In Eq. (3.106) we stated the transformation law of a vector operator [see also Eq. (2.111)]:

$$[\hat{L}_i,\hat{v}_k]=\hat{v}_j(L_i)_{jk}, \tag{3.826}$$

With the help of the above similarity transformation, we find the spherical components of the vector operator $\hat{v}_i$:

$$\hat{v}(m)\equiv\sum_{i=1}^{3}\hat{v}_i\,\langle i|1,m\rangle, \tag{3.827}$$

or, explicitly,

$$\hat{v}(\pm1)\equiv\mp\frac{1}{\sqrt{2}}(\hat{v}_1\pm i\hat{v}_2),\qquad \hat{v}(0)\equiv\hat{v}_3. \tag{3.828}$$

For these components, the commutation rules (3.826) become

$$[\hat{L}_i,\hat{v}(m)]=\sum_{m'=-1}^{1}\hat{v}(m')\langle 1,m'|\hat{L}_i|1,m\rangle. \tag{3.829}$$

They may be generalized to an arbitrary *spherical tensor operator* $\hat{v}(j,m)$ of spin j:

$$[\hat{L}_i,\hat{v}(j,m)]=\sum_{m'=-1}^{1}\hat{v}(j,m')\langle j,m'|\hat{L}_i|j,m\rangle. \tag{3.830}$$

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[23] Note that the spinor transformation laws (3.684) and (3.686) are a generalization of this relation.

For $\hat{L}_3$ and $\hat{L}_\pm$, these commutation relations become

$$[\hat{L}_3, \hat{v}(j,m)] = \hat{v}(j,m)\,m, \quad [\hat{L}_\pm, \hat{v}(j,m)] = \hat{v}(j,m\pm 1)\sqrt{(j\mp m)(j\pm m+1)}. \tag{3.831}$$

They are in one-to-one correspondence with the relations (3.782), (3.783) and (3.784) for the states $|j,m\rangle$.

For finite rotations, they give rise to the transformation behavior

$$\hat{R}\,\hat{v}(j,m)\hat{R}^{-1} = \hat{v}(j,m')D^j_{m'm}(R). \tag{3.832}$$

The use of defining such spherical tensor operators lies in the fact that all their matrix elements are related to each other by Clebsch-Gordan coefficients (3.795) via the so-called *Wigner-Eckart theorem.* Applying $\hat{v}(j,m)$ to a state $|j',m'\rangle$, we obtain a state $\hat{v}(j,m)|j',m'\rangle$, which transforms by a direct product of the representation matrices (3.800) and (3.832) like a state $|j,m;j',m'\rangle$. Its irreducible contents can be obtained with the help of the Clebsch-Gordan series (3.795). If we therefore expand

$$\hat{v}(j,m)|j',m'\rangle = \sum_{j'',m''} |j'',m''\rangle\langle j'',m''|\hat{v}(j,m)|j',m'\rangle, \tag{3.833}$$

the matrix elements $\langle j'',m''|\hat{v}(j,m)|j',m'\rangle$ must be proportional to the associated Clebsch-Gordan coefficients:

$$\langle j'',m''|\hat{v}(j,m)|j',m'\rangle = \langle j''||v(j)||j'\rangle\langle j'',m''|j,m;j',m'\rangle. \tag{3.834}$$

The proportionality constants $\langle j''||v(j)||j'\rangle$ are independent of the azimuthal quantum numbers m, m', m'', and are called the *reduced matrix elements* of the spherical tensor operator $\hat{v}(j,m)$. They vanish if j'' does not satisfy the vector coupling condition $|j-j'| \le j'' \le j+j'$.

For $j=1/2$, the matrix $d^j_{m'm}(\pi)$ is equal to $e^{-i\sigma^2\pi/2} = -i\sigma^2$. It is therefore the spin-j representation of the matrix c of (3.543), and will therefore be denoted by

$$c^{(j)} \equiv d^j_{m',m}(c) = (-1)^{j+m'}\delta_{m',-m}. \tag{3.835}$$

When applied as a similarity transformation to the representation matrix $D^j_{m'm}(\alpha,\beta,\gamma)$, we find a spin-$j$ generalization of the important 2×2 -relation (3.628):

$$[c^{(j)}]^{-1}D^j(\alpha,\beta,\gamma)c^{(j)} = D^{j*}(\alpha,\beta,\gamma). \tag{3.836}$$

The matrix $c^{(j)}$ gives rise to an invariant bilinear form for any pair of spherical tensor operators $\hat{v}(j,m)$ and $\hat{v}'(j,m)$:

$$(\hat{v},\hat{v}') \equiv \sum_{m,m'=-j}^{j} \hat{v}(j,m)c^{(j)}_{mm'}\hat{v}'(j,m') = \sum_{m=-j}^{j}(-1)^{j+m}\hat{v}(j,m)\hat{v}(j,-m). \tag{3.837}$$

This product remains invariant under rotations, since

$$D^{jT}(\alpha,\beta,\gamma)c^{(j)}D^j(\alpha,\beta,\gamma) = c^{(j)}. \tag{3.838}$$

The invariance of (3.837) is a generalization to spin-j operators of the Weyl invariance of the spinor product $\xi'_\beta c^{\beta\alpha}\xi_\alpha$ of (3.751).

For $j = 1$, the invariant product (3.837) is equivalent to the ordinary scalar product. This is seen by replacing on the right-hand side of (3.837) the spherical components $\hat{v}(1, m)$ by the cartesian ones according to (3.828), yielding

$$(\hat{v}, \hat{v}') = -\delta_{ij}\hat{v}_i\hat{v}'_j. \tag{3.839}$$

Also for $j = 1$, the spherical relation (3.838) is equivalent to the invariance of the Kronecker symbol δ_{ij} under rotations in the 3×3 defining representation:

$$R_{i_1 i'_1} R_{i_2 i'_2}\,\delta_{i'_1 i'_2} = \delta_{i_1 i_2}. \tag{3.840}$$

The invariance of scalar products (3.837) formed with $c^{(j)}$ can be used to extend the Weyl calculus to spin-j objects as follows: The spherical tensor operator $\hat{v}(j, m)$ is written as $\hat{v}\tbinom{j}{m}$, and we introduce the contravariant spherical tensor operator

$$\hat{v}\tbinom{m}{j} \equiv \sum_{m'=-j}^{j} c^{(j)}_{m,m'}\,\hat{v}\tbinom{j}{m'} = (-1)^{j+m}\,\hat{v}\tbinom{j}{-m}. \tag{3.841}$$

Then the invariant form (3.837) can simply be written as

$$(\hat{v}, \hat{v}') = \hat{v}\tbinom{j}{m}\,\hat{v}'\tbinom{m}{j}, \tag{3.842}$$

with the convention that pairs of upper and lower indices m are being summed.

The relation between the axis-angle and the Euler representation of the rotations on the two sides of (3.798) is easily found using the explicit 2×2 -representation (3.423) in the axis-angle form, and in the Euler form

$$\begin{aligned} & e^{-i\alpha\sigma^3/2}e^{-i\beta\sigma^2/2}e^{-i\gamma\sigma^3/2} \\ &= \left(\cos\frac{\alpha}{2} - i\sigma^3\sin\frac{\alpha}{2}\right)\left(\cos\frac{\beta}{2} - i\sigma^2\sin\frac{\beta}{2}\right)\left(\cos\frac{\gamma}{2} - i\sigma^3\sin\frac{\gamma}{2}\right) \\ &= \cos\frac{\beta}{2}\cos\frac{\alpha+\gamma}{2} + \sin\frac{\beta}{2}\frac{\alpha-\gamma}{2}i\sigma^1 \\ &\quad -\sin\frac{\beta}{2}\cos\frac{\alpha-\gamma}{2}i\sigma^2 - \sin\frac{\beta}{2}\sin\frac{\alpha+\gamma}{2}i\sigma^3. \end{aligned} \tag{3.843}$$

Comparing the coefficients gives

$$\begin{aligned} \cos\frac{\varphi}{2} &= \cos\frac{\beta}{2}\cos\frac{\alpha+\gamma}{2}, \\ \hat{\boldsymbol{\varphi}}\sin\frac{\varphi}{2} &= \left(-\sin\frac{\alpha-\gamma}{2}, \cos\frac{\alpha-\gamma}{2}, \sin\frac{\alpha+\gamma}{2}\right)\sin\frac{\beta}{2}. \end{aligned} \tag{3.844}$$

More details on the rotation group can be found in the textbook by Edmonds quoted in Notes and References.

Lorentz Group

To extend these results to the Lorentz group we make use of the fact that due to the decompositions (3.788) and (3.789), pure rotations can be decomposed as

$$e^{-i\boldsymbol{\varphi}\cdot\hat{\mathbf{L}}} = e^{-i\boldsymbol{\varphi}\cdot\hat{\mathbf{J}}^{(1)}} e^{-i\boldsymbol{\varphi}\cdot\hat{\mathbf{J}}^{(2)}}, \tag{3.845}$$

where $\mathbf{J}^{(1)}$ and $\mathbf{J}^{(2)}$ are the matrices (3.785). The pure Lorentz transformations are

$$e^{-i\boldsymbol{\zeta}\cdot\hat{\mathbf{M}}} = e^{-\boldsymbol{\zeta}\cdot\hat{\mathbf{J}}^{(1)}} e^{\boldsymbol{\zeta}\cdot\hat{\mathbf{J}}^{(2)}}, \tag{3.846}$$

with $e^{-\boldsymbol{\zeta}\cdot\hat{\mathbf{J}}^{(1)}} e^{\boldsymbol{\zeta}\cdot\hat{\mathbf{J}}^{(2)}}$ having again matrix elements of rotations, as calculated above. Thus, given the parameters $\boldsymbol{\varphi}$ and $\boldsymbol{\zeta}$ of the Lorentz transformation in question, we merely have to find the corresponding Euler angles and take the corresponding rotation matrices from (3.800) and (3.809).

Note that for pure Lorentz transformations the rotation parameters are imaginary so that the trigonometric functions become hyperbolic. For pure Lorentz transformations with imaginary angles, the relation between the axis-angle and the Euler representations corresponding to the two sides of (3.798) is then given by relations like (3.844), but with cosine and sine functions continued to the corresponding hyperbolic forms.

3.19 HIGHER-SPIN FIELDS

The construction of invariant actions can be generalized to fields of arbitrary spin. If we restrict ourselves to those representations which contain only one spin, the situation is very similar to the spin-1/2 case: There are two spinor fields of the Weyl type ξ_α and $\eta^{\dot\beta}$, transforming according to the $D^{(s,0)}$ and $D^{(0,s)}$-representations, respectively

$$\begin{aligned} \xi(x) \xrightarrow{\Lambda} \xi'_{\alpha'}(x') &= D^{(s,0)}(\Lambda)_{\alpha'}{}^{\alpha}\xi_\alpha(x), \\ \eta(x) \xrightarrow{\Lambda} \eta'^{\dot\beta'}(x') &= D^{(0,s)}(\Lambda)^{\dot\beta'}{}_{\dot\beta}\eta^{\dot\beta}(x). \end{aligned} \tag{3.847}$$

Now, according to the last section, the matrices $D^{(s,0)}(\Lambda)$ are just the symmetrized direct products of $2s$ representations $D^{(\frac{1}{2},0)}(\Lambda)$. They satisfy the same relation as $D^{(\frac{1}{2},0)}$ itself:

$$D^{(s,0)}(\Lambda) = D^{(0,s)}(\Lambda)^{-1}. \tag{3.848}$$

Hence

$$\xi^\dagger\eta \ , \ \eta^\dagger\xi \tag{3.849}$$

are the only Lorentz-invariant invariant bilinear combinations of the spinor fields. What about invariants involving derivatives? For this we recall that in the spin-$\frac{1}{2}$ case

$$\xi^\dagger i\tilde\sigma^\mu\partial_\mu\xi \ , \ \eta^\dagger i\sigma^\mu\partial_\mu\eta \tag{3.850}$$

were invariant due to the property (3.436). The invariance remains true for a product of $2s$ factors whose right and left indices are symmetrized. Therefore

$$\xi^\dagger(i^{2s}\tilde{\sigma}^{\mu_1}\times\ldots\times\tilde{\sigma}^{\mu_{2s}}\partial_{\mu_1}\cdots\partial_{\mu_{2s}})\xi\equiv\xi^\dagger(\tilde{\sigma}i\partial)^{\{2s\}}\xi \tag{3.851}$$

and

$$\eta^\dagger(i^{2s}\sigma^{\mu_1}\times\ldots\times\sigma^{\mu_{2s}}\partial_{\mu_1}\cdots\partial_{\mu_{2s}})\eta\equiv\eta^\dagger(\sigma i\partial)^{\{2s\}}\eta \tag{3.852}$$

are invariants, where the curly brackets indicate the symmetrization of the indices. We may therefore write the action as

$$\mathcal{A}=\int d^4x\left\{\xi^\dagger(\tilde{\sigma}i\partial)^{\{2s\}}\xi+\eta^\dagger(\sigma i\partial)^{\{2s\}}\eta-M_1^{2s}\xi^\dagger\eta-M_2^{2s}\eta^\dagger\xi\right\}. \tag{3.853}$$

In the absence of the mass terms, each of the derivative pieces gives by itself an invariant action which maximally violates parity. This fact will be needed to explain the maximal parity violation in weak interactions briefly discussed on p. 182. The equations of motion (3.441) and (3.442) become

$$(\tilde{\sigma}i\partial)^{\{2s\}}\xi(x) = M_1^{2s}\eta(x), \tag{3.854}$$

$$(\sigma i\partial)^{\{2s\}}\eta(x) = M_2^{2s}\xi(x). \tag{3.855}$$

They can be inserted into each other to give

$$(\tilde{\sigma}i\partial)^{\{2s\}}(\sigma i\partial)^{\{2s\}}\left\{\begin{array}{c}\xi(x)\\ \eta(x)\end{array}\right\}=M_1^{2s}M_2^{2s}\left\{\begin{array}{c}\xi(x)\\ \eta(x)\end{array}\right\}. \tag{3.856}$$

The left-hand side contains a product of two symmetrized products. Since each $2s$ factors are symmetric under simultaneous exchange of left and right indices, we can omit the symmetrization in the contracted indices, and use in each of them relation (3.444) to derive

$$[(\tilde{\sigma}i\partial)(\sigma i\partial)]^{\{2s\}}=(-\partial^2 1)^{\{2s\}}=(-\partial^2)^{2s}(1)^{\{2s\}}, \tag{3.857}$$

with $(1)^{\{2s\}}$ being the unit matrix in the symmetrized subspace. In momentum space, this amounts to the mass shell relation

$$(p^2)^{2s}=M_1^{2s}M_2^{2s}=(M^2)^{2s}. \tag{3.858}$$

As in the spin-1/2 case, space inversion changes $\partial\rightarrow\tilde{\partial}$ and the representation matrices

$$D^{(s,0)}(\Lambda)\rightarrow D^{(0,s)}(\Lambda). \tag{3.859}$$

If one wants to have a representation space of the Lorentz group including space inversions, one must combine the two spinors $\xi(x)$ and $\eta(x)$ into a bispinor with $2\times(2s+1)$ components

$$\psi(x)=\left(\begin{array}{c}\xi(x)\\ \eta(x)\end{array}\right). \tag{3.860}$$

On this space, parity is represented as in (3.484) by

$$\psi(x) \xrightarrow{P} \psi'_P(x) = D(P)\psi(\tilde{x}), \tag{3.861}$$

with a representation matrix which looks like (3.485), but contains now four blocks of $(2s+1) \times (2s+1)$ -matrices:

$$D(P) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \eta_P \gamma_0. \tag{3.862}$$

It is obvious that this matrix changes the generators **L** and **M** of the Lorentz group in the spin-s representation as in Eqs. (3.483).

Invariance under space inversion requires

$$M_1 = M_2 = M^{2s}, \tag{3.863}$$

and thus the presence of both derivative terms in (3.853). There are now generalized γ-matrices with

$$(\gamma i\partial)^{\{2s\}} = \begin{pmatrix} 0 & (\sigma i\partial)^{\{2s\}} \\ (\tilde{\sigma} i\partial)^{\{2s\}} & 0 \end{pmatrix}, \tag{3.864}$$

and we can write down a parity-invariant action for the bispinors $\psi(x)$ as

$$\mathcal{A} = \int d^4x\, \bar{\psi}(x) \left[(\gamma i\partial)^{\{2s\}} - M^{2s}\right] \psi(x), \tag{3.865}$$

where

$$\bar{\psi}(x) \equiv \begin{pmatrix} \eta^\dagger \\ \xi^\dagger \end{pmatrix} = \psi^\dagger(x)(\gamma^0)^{\{2s\}}. \tag{3.866}$$

The field equation is

$$\left[(\gamma i\partial)^{\{2s\}} - M^{2s}\right] \psi(x) = 0. \tag{3.867}$$

3.19.1 Plane-Wave Solutions

One can easily write down plane wave solutions of the spin-s wave equation (3.867):

$$\mathrm{f}_{\mathbf{p}\,s_3}(x) \equiv u(\mathbf{p}, s_3)\frac{e^{-ipx}}{\sqrt{Vp^0/M}}, \qquad \mathrm{f}^c_{\mathbf{p}\,s_3}(x) \equiv v(\mathbf{p}, s_3)\frac{e^{ipx}}{\sqrt{Vp^0/M}}, \tag{3.868}$$

where $u(\mathbf{p}, s_3)$ and $v(\mathbf{p}, s_3)$ are the positive- and negative-energy solutions of momentum $\mathbf{p}$ and $-\mathbf{p}$, respectively. satisfying the generalized Dirac equations in momentum space

$$(\not{p}^{\{2s\}} - M)u(\mathbf{p}, s_3) = 0, \qquad (\not{p}^{\{2s\}} + M)u(\mathbf{p}, s_3) = 0. \tag{3.869}$$

The second can be obtained from the first via a relation like (3.617):

$$v(\mathbf{p}, s_3) = C\bar{u}^T(\mathbf{p}, s_3). \tag{3.870}$$

Here C is the charge conjugation matrix for arbitrary spin

$$C = \gamma^{\{2s\}\,0} = \begin{pmatrix} c^{\{2s\}} & 0 \\ 0 & c^{\{2s\}} \end{pmatrix}. \tag{3.871}$$

The matrices $c^{\{2s\}}0$ are equivalent to the matrices $c^{(s)}$ introduced in Eq. (3.835). They have the important property that

$$c^{\{2s\}} = (-1)^{2s}. \tag{3.872}$$

The rest spinors $\chi^{\{2s\}}(s_3)$ have symmetrized labels 1/2 and −1/2. These are uniquely specified by the number n_1 of up-spins and n_2 of down-spins, which are the labels of the basis vectors $|n_1, n_2)$ in Eq. (3.772). Thus we may write $\chi^{\{2s\}}(s_3)$ more explicitly as $\chi^{\{2s\}}_{n_1,n_2}(s_3)$. The label s_3 specifies the eigenvalues of the third component of angular momentum, and corresponds to the label m of the basis vectors (3.781). Hence

$$\chi^{\{2s\}}_{n_1,n_2}(s_3) = \delta_{s_3,(n_1-n_2)/2}, \qquad n_1 + n_2 = 2s. \tag{3.873}$$

These spinors satisfy the obvious completeness relation

$$\sum_{s_3} \chi^{\{2s\}}_{n_1,n_2}(s_3)\chi^{\{2s\}*}_{n_1',n_2'}(s_3) = \delta_{n_1,n_2} \tag{3.874}$$

Using this, we find for the spinors $u^{\{2s\}}(\mathbf{p}, s_3)$ a polarization sum [compare (3.644)]

$$P(p) \equiv \sum_{s_3} u^{\{2s\}}(\mathbf{p}, s_3)u^{\{2s\}*}(\mathbf{p}, s_3) = \left(\frac{M + p\sigma^{\{2s\}}}{2M}\right)^{\{2s\}}. \tag{3.875}$$

It is a straigthforward generalization of the Dirac case. The polarization sums for the spinors $v^{\{2s\}}(\mathbf{p}, s_3)$ can be calculated similarly.

From the spinors $w^{2s}(\mathbf{p}, s_3)$ we form the mirror-reflected spinors $w^{2s}(-\mathbf{p}, s_3)$

$$w^{\{2s\}}(\tilde{\mathbf{p}}, s_3) = B^{\{2s\}}_{\tilde{\mathbf{p}}}(\zeta)\chi^{\{2s\}}(s_3) = \sqrt{\frac{\tilde{p}\sigma}{M}}^{\{2s\}}, \tag{3.876}$$

and after multiplication with the generalized charge-conjugation matrix c^{2s} we combining both spinors to bispinors $u^{2s}(\mathbf{p}, s_3)$ and $v^{2s}(\mathbf{p}, s_3)$ of particle and antiparticles of spin s.

3.20 VECTOR FIELD AS A HIGHER-SPIN FIELD

Some remarks are in order concerning the fields transforming according to the representation $D^{(s_1,s_2)}(\Lambda)$ with both $s_1, s_2 \neq 0$ which were omitted in the above construction. The most prominent among them is the spinor field with $s_1 = s_2 = \frac{1}{2}$ which we denote by ${\xi_\alpha}^{\dot\beta}(x)$. It is this field which is equivalent to a vector field $A^\mu(x)$, which was discussed before separately in Section (3.6) in the massless case (for the massive case see Section 5.5). To see this equivalence we observe first of all, that both representations have a spin content 0 and 1. For the spinor ${\xi_\alpha}^{\dot\beta}(x)$ this follows from the addition rule of angular momenta (3.796). In the vector field $A_\mu(x)$, the zeroth component transforms according to the spin-0 representation, the spatial components according to the spin-1 representation of the rotation group.

There exists a simple relation between the two fields. The spinor field transforms according to the $\left(\frac{1}{2}, \frac{1}{2}\right)$ representation of the Lorentz group as follows:

$$\begin{aligned} \xi \xrightarrow{\Lambda} {\xi'(x')_{\alpha'}}^{\dot\beta'} &= {D^{(\frac{1}{2},0)}(\Lambda)_{\alpha'}}^{\alpha}\, {D^{(0,\frac{1}{2})}(\Lambda)^{\dot\beta'}}_{\dot\beta}\, {\xi_\alpha}^{\dot\beta}(x) \\ &= {\left[D^{(\frac{1}{2},0)}(\Lambda)\xi(x)D^{(0,\frac{1}{2})T}(\Lambda)\right]_{\alpha'}}^{\dot\beta'}. \end{aligned} \tag{3.877}$$

The 2×2 components of the spinor can be mapped into the four components of a vector by forming

$$\xi^\mu(x) \equiv c_{\dot\beta\dot\beta'}\tilde\sigma^{\mu\,\dot\beta'\alpha}{\xi_\alpha}^{\dot\beta}(x) = \mathrm{tr}\,[c\tilde\sigma^\mu\xi(x)]. \tag{3.878}$$

Using the Lorentz transformation rules of Section 3.17 it is easy to verify that $\xi^\mu(x)$ transforms indeed like the vector field $A^\mu(x)$ in Eq. (3.267):

$$\begin{aligned} \xi^\mu(x) \xrightarrow{\Lambda} \xi'^\mu(x') &= \mathrm{tr}\,\left[c\tilde\sigma^\mu D^{(\frac{1}{2},0)}(\Lambda)\xi(x)D^{(0,\frac{1}{2})T}(\Lambda)\right] \\ &= \mathrm{tr}\,\left[c(c^{-1}D^{(0,\frac{1}{2})T}(\Lambda)c)\tilde\sigma^\mu D^{(\frac{1}{2},0)}(\Lambda)\xi(x)\right]. \end{aligned} \tag{3.879}$$

Now we make use of the relation (3.622) to set

$$c^{-1}\sigma^{\mu T}c = -\sigma^\mu, \quad c^{-1}D^{(0,\frac{1}{2})T}(\Lambda)c = D^{(\frac{1}{2},0)^\dagger}(\Lambda), \tag{3.880}$$

and to rewrite (3.879) as

$$\xi'^\mu(x') = \mathrm{tr}\,\left[cD^{(\frac{1}{2},0)^\dagger}(\Lambda)\tilde\sigma^\mu D^{(\frac{1}{2},0)}(\Lambda)\xi(x)\right]. \tag{3.881}$$

With the help of (3.436) we obtain now the vector property of the composite field $\xi^m(x)$:

$$\xi'^\mu(x') = {\Lambda^\mu}_\nu\,\mathrm{tr}\,[c\tilde\sigma^\nu\xi(x)] = {\Lambda^\mu}_\nu\,\xi^\nu(x), \tag{3.882}$$

so that $\xi^\mu(x)$ transforms indeed like $A^\mu(x)$ in (3.267).

A special feature of all representations $D^{(s,s')}$ with $s = s'$ is that they are invariant under space inversions since this interchanges s and s'. Thus no doubling of fields is needed to accommodate space inversions. In the vector form of the $\left(\frac{1}{2}, \frac{1}{2}\right)$ representation this was seen before in the transformation law (3.283).

3.21 RARITA SCHWINGER FIELD FOR SPIN 3/2

Another frequently-encountered form of higher spin fields which is not of the $(s, 0) + (0, s)$ type is due to Rarita and Schwinger and describes spin-3/2 particles. It combines vector and bispinor properties and is written as $\psi_{\mu a}(x)$, thus transforming according to

$$\psi_{\mu a}(x) \xrightarrow{\Lambda} \psi'_{\mu a}(x') = \Lambda_\mu{}^\nu \begin{pmatrix} D^{(\frac{1}{2},0)}(\Lambda) & 0 \\ 0 & D^{(0,\frac{1}{2})}(\Lambda) \end{pmatrix}_{ab} \psi_{\nu b}(x). \tag{3.883}$$

Group theoretically speaking, this is a direct product of the representations $\left(\frac{1}{2}, \frac{1}{2}\right)$ (for the index μ) and $\left(\frac{1}{2}, 0\right) + \left(0, \frac{1}{2}\right)$ (for the index a).

We can employ the usual rules for the addition of angular momentum and apply them to $\mathbf{J}^{(1)}$ and $\mathbf{J}^{(2)}$ in (3.788). Then the direct product of two representations

$$D^{(s_1,s_2)} \times D^{(s'_1,s'_2)} \tag{3.884}$$

must have the following irreducible contents

$$\begin{aligned} &D^{(|s_1-s_2|,|s'_1-s'_2|)} + D^{(|s_1-s_2|,|s'_1-s'_2|+1)} + \ldots + D^{(|s_1-s_2|,s'_1+s'_2)} \\ &+ D^{|s_1-s_2|+1,|s'_1-s'_2|)} + D^{(|s_1-s_2|+1,|s'_1-s'_2|+1)} + \ldots + D^{(|s_1-s_2|+1,s'_1+s'_2)} \\ &+ \ldots \\ &+ D^{(s_1+s_2,|s'_1-s'_2|)} + D^{(s_1+s_2,|s'_1-s'_2|+1)} + \ldots + D^{(s_1+s_2,s'_1+s'_2)}. \end{aligned}$$

In this expansion, the spins s_1 and s_2 of of $\mathbf{J}^{1,2}$ combine to all spins from $|s_1 - s_2|$ to $s_1 + s_2$ [recall (3.796)], and similarly s'_1 and s'_2 to all spins from $|s'_1 - s'_2|$ to $s'_1 + s'_2$. Therefore $\psi_{\mu a}$ is equivalent to a sum of $D^{(s_1,s_2)}$ representations:

$$\left(0, \frac{1}{2}\right) + \left(1, \frac{1}{2}\right) + \left(\frac{1}{2}, 0\right) + \left(\frac{1}{2}, 1\right). \tag{3.885}$$

Remember that the symmetry with respect to the interchange $s_1 \leftrightarrow s_2$ is necessary for a parity-invariant Lagrangian. Now, if we want to describe only a spin-3/2 particle, the representations $\left(0, \frac{1}{2}\right)$ and $\left(\frac{1}{2}, 0\right)$ are superfluous and have to be projected out. This can be done by a constraint analogous to the Lorentz condition for the electromagnetic field:

$$\partial^\mu \psi_{\mu a} = 0. \tag{3.886}$$

Obviously, this derivative transforms like $\left(0, \frac{1}{2}\right) + \left(\frac{1}{2}, 0\right)$ and has only a spin-1/2 content, which is therefore removed from (3.885). It remains to make sure that the representation $\left(1, \frac{1}{2}\right) + \left(\frac{1}{2}, 1\right)$ in $\psi_{\mu a}$ describes only a spin-3/2 particle. This is achieved by another condition on the field:

$$\gamma^\mu{}_{ab} \psi_{\mu b} = 0. \tag{3.887}$$

This projection of the field transforms once more like $\left(0,\frac{1}{2}\right)+\left(\frac{1}{2},0\right)$, and setting it equal to zero eliminates one more spin-$\frac{1}{2}$ degree of freedom thus ensuring the survival of only the spin-3/2 content in $\psi_{\mu a}$.

It remains to construct an invariant action with the property that the equations of motion automatically ensure the constraints (3.886), (3.887). There are now several possible invariants which can be used. If we allow at most for one derivative we may combine

$$\bar{\psi}^\mu i\gamma^\nu\partial_\nu\psi_\mu,\quad \bar{\psi}_\mu\gamma^\mu\partial^\nu\psi_\nu,\quad \bar{\psi}_\mu\gamma^\nu\partial^\mu\psi_\nu,\quad \bar{\psi}_\mu\gamma^\mu\gamma^\nu\psi_\nu,\quad \bar{\psi}^\mu\psi_\mu. \tag{3.888}$$

The most general combination which leads to a hermitian action of a pure spin-3/2 particle can be shown to be[24]

$$\mathcal{A}=\int d^4x\,\mathcal{L}(x)=\int d^4x\,\bar{\psi}_\mu(x)L^{\mu\nu}(i\partial)\psi_\nu(x), \tag{3.889}$$

where $L^{\mu\nu}(i\partial)$ is the differential operator

$$\begin{aligned} L^{\mu\nu}(i\partial) \;=\; & (i\partial\!\!\!/-M)g^{\mu\nu}+w\,\gamma^\mu i\partial^\nu+w^*\gamma^\nu\partial^\mu \\ & +\frac{1}{2}(3ww^*+w+w^*+1)\gamma^\mu i\partial\!\!\!/\gamma^\nu \\ & +M\left[3ww^*+\frac{3}{2}(w+w^*)+1\right]\gamma^\mu\gamma^\nu, \end{aligned} \tag{3.890}$$

where w is an arbitrary complex number. The equations of motion are given by

$$L^{\mu\nu}(i\partial)\psi_\nu(x)=0. \tag{3.891}$$

It can easily be verified that a field $\psi_{\mu a}(x)$ which satisfies the constraints (3.886), (3.887) solves (3.891) if and only if the Dirac equation is fulfilled separately for each vector index μ:

$$(i\partial\!\!\!/-M)_a{}^{a'}\psi_{\mu a'}(x)=0, \tag{3.892}$$

showing that the particle has mass M. Some algebra is necessary to show that the constraints (3.886), (3.887) follow from (3.891). For this we go to momentum space and contract $L^{\mu\nu}(p)\psi_\nu(p)=0$ once with γ_μ and once with p_μ, using the relations $\gamma_\mu p\!\!\!/=-p\!\!\!/\gamma_\mu+2p_\mu$ and $\gamma^\mu\gamma_\mu=4$. The two contractions yield $\gamma^\mu\psi_\mu=0$ and $p^\mu\psi_\mu=0$, which are a direct consequence of the anticommutation rules (3.450).

Appendix 3A Derivation of Baker-Campbell-Hausdorff Formula

The standard Baker-Campbell-Hausdorff formula, from which our formula (3.70) can be derived, reads

$$e^{\hat{A}}e^{\hat{B}}=e^{\hat{C}}, \tag{3A.1}$$

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[24] See Notes and References for literature.

where

$$\hat{C} = \hat{B} + \int_0^1 dtg(e^{\mathrm{ad}A\,t}e^{\mathrm{ad}B})[\hat{A}]. \tag{3A.2}$$

Here $g(z)$ is the function

$$g(z) \equiv \frac{\log z}{z-1} = \sum_{n=0}^{\infty} \frac{(1-z)^n}{n+1} \tag{3A.3}$$

and $\mathrm{ad}B$ is the operator associated with $\hat{B}$ in the so-called *adjoint representation*, which is defined by

$$\mathrm{ad}B[\hat{A}] \equiv [\hat{B}, \hat{A}]. \tag{3A.4}$$

One also defines the trivial adjoint operator $(\mathrm{ad}B)^0[\hat{A}] = 1[\hat{A}] \equiv \hat{A}$. By expanding the exponentials in Eq. (3A.2) and using the power series (2A.3), one finds the explicit formula

$$\begin{aligned}\hat{C} = \hat{B} + \hat{A} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n+1} &\sum_{p_i,q_i;p_i+q_i\geq 1} \frac{1}{1+\sum_{i=1}^n p_i} \\ &\times \frac{(\mathrm{ad}A)^{p_1}}{p_1!}\frac{(\mathrm{ad}B)^{q_1}}{q_1!}\cdots\frac{(\mathrm{ad}A)^{p_n}}{p_n!}\frac{(\mathrm{ad}B)^{q_n}}{q_n!}[\hat{A}].\end{aligned} \tag{3A.5}$$

The lowest expansion terms are

$$\begin{aligned}\hat{C} &= \hat{B} + \hat{A} - \frac{1}{2}\left[\tfrac{1}{2}\mathrm{ad}A + \mathrm{ad}B + \tfrac{1}{6}(\mathrm{ad}A)^2 + \tfrac{1}{2}\mathrm{ad}A\,\mathrm{ad}B + \tfrac{1}{2}(\mathrm{ad}B)^2 + \ldots\right][\hat{A}] \\ &\quad + \frac{1}{3}\left[\tfrac{1}{3}(\mathrm{ad}A)^2 + \tfrac{1}{2}\mathrm{ad}A\,\mathrm{ad}B + \tfrac{1}{2}\mathrm{ad}B\mathrm{ad}A + (\mathrm{ad}B)^2 + \ldots\right][\hat{A}] \\ &= \hat{A} + \hat{B} - \frac{1}{2}[\hat{B}, \hat{A}] + \frac{1}{12}([\hat{A}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{B}, \hat{A}]]) + \ldots\ .\end{aligned} \tag{3A.6}$$

To prove this, we derive and solve a differential equation for the function

$$\hat{C}(t) = \log(e^{\hat{A}t}e^{\hat{B}}), \tag{3A.7}$$

and obtain the desired operator $\hat{C}$ from its value at $t = 1$, $\hat{C} = \hat{C}(1)$. The starting point is the observation that for any $\hat{M}$,

$$e^{\hat{C}(t)}\hat{M}e^{-\hat{C}(t)} = e^{\mathrm{ad}C(t)}[\hat{M}], \tag{3A.8}$$

by definition of $\mathrm{ad}C$. The left-hand side can also be rewritten as

$$e^{\hat{A}t}e^{\hat{B}}\hat{M}e^{-\hat{B}}e^{-\hat{A}t} = e^{\mathrm{ad}A\,t}e^{\mathrm{ad}B}[\hat{M}], \tag{3A.9}$$

so that we have

$$e^{\mathrm{ad}C(t)} = e^{\mathrm{ad}A\,t}e^{\mathrm{ad}B}. \tag{3A.10}$$

Differentiation of (3A.7) shows that

$$e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -\hat{A}. \tag{3A.11}$$

The left-hand side, on the other hand, can be rewritten in general as

$$e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)], \tag{3A.12}$$

where

$$f(z) \equiv \frac{e^z-1}{z}. \tag{3A.13}$$

This will be verified below. It implies that

$$f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)] = \hat{A}. \tag{3A.14}$$

We now define the function $g(z)$ as in (3A.3) and see that it satisfies

$$g(e^z)f(z) \equiv 1. \tag{3A.15}$$

We therefore have the trivial identity

$$\dot{\hat{C}}(t) = g(e^{\mathrm{ad}C(t)})f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)]. \tag{3A.16}$$

Using (3A.14) and (3A.10), this turns into the differential equation

$$\dot{\hat{C}}(t) = g(e^{\mathrm{ad}C(t)})[\hat{A}] = e^{\mathrm{ad}A\,t}e^{\mathrm{ad}B}[\hat{A}], \tag{3A.17}$$

from which we find directly the result (3A.2).

To complete the proof we must verify (3A.12). For this consider the operator

$$\hat{O}(s,t) \equiv e^{\hat{C}(t)s}\frac{d}{dt}e^{-\hat{C}(t)s}. \tag{3A.18}$$

Differentiating this with respect to s gives

$$\begin{aligned}\partial_s\hat{O}(s,t) &= e^{\hat{C}(t)s}\hat{C}(t)\frac{d}{dt}\left(e^{-\hat{C}(t)s}\right) - e^{\hat{C}(t)s}\frac{d}{dt}\left(\hat{C}(t)e^{-\hat{C}(t)s}\right)\\ &= -e^{\hat{C}(t)s}\dot{\hat{C}}(t)e^{-\hat{C}(t)s}\\ &= -e^{\mathrm{ad}C(t)s}[\dot{\hat{C}}(t)].\end{aligned} \tag{3A.19}$$

Hence

$$\begin{aligned}\hat{O}(s,t)-\hat{O}(0,t) &= \int_0^s ds'\partial_{s'}\hat{O}(s',t)\\ &= -\sum_{n=0}^{\infty}\frac{s^{n+1}}{(n+1)!}\left(\mathrm{ad}C(t)\right)^n[\dot{\hat{C}}(t)],\end{aligned} \tag{3A.20}$$

from which we obtain

$$\hat{O}(1,t) = e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)], \tag{3A.21}$$

which is what we wanted to prove.

Note that the final form of the series for $\hat{C}$ in (3A.6) can be rearranged in many different ways, using the Jacobi identity for the commutators. It is a nontrivial task to find a form involving the smallest number of terms.[25]

Appendix 3B Wigner Rotations and Lobatschewski Geometry of Rapidities

Here we calculate the Wigner rotation responsible for the Thomas precession. Expressing (3.690) infinitesimally, we write the small rotation $e^{-i\Delta\alpha\sigma/2}$ as

$$R(t) \equiv e^{-id\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}\,dt/2} = e^{\boldsymbol{\zeta}(t+dt)\cdot\boldsymbol{\sigma}/2}e^{-d\boldsymbol{\epsilon}\cdot\boldsymbol{\sigma}/2}e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2} = B^{-1}(\boldsymbol{\zeta}(t+dt))B(d\boldsymbol{\epsilon})B(\boldsymbol{\zeta}). \tag{3B.1}$$

The pure rotation character of the product on the right-hand side is obvious, since a particle in its rest frame is transformed by three boost transformations back to the rest frame. Being a small rotation, the left-hand side has necessarily the form

$$R = 1 - i\dot{\boldsymbol{\alpha}}\cdot\boldsymbol{\sigma}dt/2, \tag{3B.2}$$

where $\boldsymbol{\Omega} = -\boldsymbol{\alpha}$ is an angular velocity describing precession rate defined by $\dot{\boldsymbol{\sigma}} = R\boldsymbol{\sigma}R^{-1} = \boldsymbol{\Omega}\times\boldsymbol{\sigma}$. The parameter $d\boldsymbol{\zeta}$ of the infinitesimal Lorentz transformation in (3B.1) must be chosen such that the final laboratory rapidity is $\boldsymbol{\zeta} + d\boldsymbol{\zeta}$. Obviously, $d\boldsymbol{\zeta}$ is the change in rapidity as seen by the moving electron, whereas

$$B^{-1}(\boldsymbol{\epsilon})B(d\boldsymbol{\zeta})B(\boldsymbol{\zeta}) \tag{3B.3}$$

determines the change in velocity as seen in the laboratory. Let us set this equal to

$$R(d\boldsymbol{\alpha}')B(d\boldsymbol{\zeta}'). \tag{3B.4}$$

Then we can expand (3B.1) up to first order in $d\boldsymbol{\zeta}$:

$$\begin{aligned} R &= B^{-1}(\boldsymbol{\zeta}(t+dt))B(\boldsymbol{\zeta})R(d\boldsymbol{\alpha}')B(d\boldsymbol{\epsilon}) \\ &= 1 + \dot{B}(-\boldsymbol{\zeta})B(\boldsymbol{\zeta})dt + [R(d\boldsymbol{\alpha}') - 1] + [B(d\boldsymbol{\zeta}') - 1]. \end{aligned} \tag{3B.5}$$

It is straightforward to calculate the second term in the notation (3.416) in natural units with $c = 1$: where

$$B_{\hat{\boldsymbol{\zeta}}}(\zeta) = \frac{1}{\sqrt{2(\gamma+1)}}(\gamma + 1 - \gamma\mathbf{v}\cdot\boldsymbol{\sigma}). \tag{3B.6}$$

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[25] For a recent discussion see J.A. Oteo, J. Math. Phys. *32*, 419 (1991).

and

$$\dot{B}_{\hat{\zeta}}(-\zeta) = -\frac{\dot{\gamma}}{2(\gamma+1)}B_{\hat{\zeta}}(-\zeta) + \frac{1}{\sqrt{2(\gamma+1)}}\left[\dot{\gamma}\left(1+\mathbf{v}\cdot\boldsymbol{\sigma}\right)+\gamma\dot{\mathbf{v}}\cdot\boldsymbol{\sigma}\right] \tag{3B.7}$$

After multiplying this with $\dot{B}_{\hat{\zeta}}(\zeta)$ we obtain

$$\dot{B}_{\hat{\zeta}}(-\zeta)B_{\hat{\zeta}}(\zeta) = -\frac{\dot{\gamma}}{2(\gamma+1)}+\frac{1}{2(\gamma+1)}\left[\dot{\gamma}\left(1+\mathbf{v}\cdot\boldsymbol{\sigma}\right)+\gamma\dot{\mathbf{v}}\cdot\boldsymbol{\sigma}\right]\left(\gamma+1-\gamma\mathbf{v}\cdot\boldsymbol{\sigma}\right). \tag{3B.8}$$

The sum of all terms without any factor $\boldsymbol{\sigma}$ cancel each other since they are equal to

$$-\frac{\dot{\gamma}}{2(\gamma+1)}+\frac{\dot{\gamma}}{2}-\frac{1}{2(\gamma+1)}\left[\dot{\gamma}\gamma\,v^2+\gamma^2\mathbf{v}\cdot\dot{\mathbf{v}}\right], \tag{3B.9}$$

which can be simplified using the trivial identities

$$\dot{\gamma}=\mathbf{v}\cdot\dot{\mathbf{v}}\,\gamma^3, \qquad v^2=\frac{\gamma^2-1}{\gamma^2}. \tag{3B.10}$$

to

$$-\frac{\dot{\gamma}}{2(\gamma+1)}+\frac{\dot{\gamma}}{2}-\frac{\dot{\gamma}\gamma}{2(\gamma+1)}\dot{\gamma}\gamma\left[v^2+\frac{1}{\gamma^2}\right]=0. \tag{3B.11}$$

Using the identity (3.692), the remaining terms can be decomposed as follows:

$$\dot{B}_{\hat{\zeta}}(-\zeta)B_{\hat{\zeta}}(\zeta)=-\dot{\boldsymbol{\beta}}\cdot\boldsymbol{\sigma}/2-i\,\dot{\boldsymbol{\alpha}}\cdot\boldsymbol{\sigma}/2, \tag{3B.12}$$

where

$$\dot{\boldsymbol{\beta}}=\frac{1}{(\gamma+1)}\left[-\dot{\gamma}\,\mathbf{v}-\gamma(\gamma+1)\dot{\mathbf{v}}\right]=-\gamma^2\dot{\mathbf{v}}_{\parallel}-\gamma\dot{\mathbf{v}}_{\perp}, \tag{3B.13}$$

is found with the help of (3B.10). The vectors $\dot{\mathbf{v}}_{\parallel}$ and $\dot{\mathbf{v}}_{\perp}$ denote the projections of $\dot{\mathbf{v}}$ parallel and orthogonal to $\mathbf{v}$, respectively. The parameter $\dot{\boldsymbol{\alpha}}$ is found to be

$$\dot{\boldsymbol{\alpha}}=\frac{\gamma^2}{(\gamma+1)}\dot{\mathbf{v}}\times\mathbf{v}. \tag{3B.14}$$

The first, hermitian term in (3B.12) corresponds in (3B.5) to a pure infinitesimal Lorentz transformation. Since the final result (3B.5) must be a pure rotation, this term must be canceled by the last term in (3B.5) which is also hermitian. Thus we conclude that

$$B(d\boldsymbol{\zeta}')=1-\frac{1}{2}\left(\gamma^2\dot{\mathbf{v}}_{\parallel}+\gamma\,\dot{\mathbf{v}}_{\perp}\right)\cdot\boldsymbol{\sigma}\,dt. \tag{3B.15}$$

The remaining antihermitian term is of the type (3B.2) and gives a first contribution to the angular velocity of Thomas precession (after reinserting here the omitted light velocity c):

$$\boldsymbol{\Omega}_1=\frac{1}{c^2}\frac{\gamma^2}{\gamma+1}(\dot{\mathbf{v}}\times\mathbf{v}). \tag{3B.16}$$

This generalizes the approximate formula (3.697) to finite velocities $\mathbf{v}$, and proves the earlier-stated result (3.699).

In order to find the second contribution to the angular velocity we must calculate the second term in (3B.5) $R(d\boldsymbol{\alpha}') - 1$. Thus we transform $B(d\boldsymbol{\epsilon}) = 1 - d\boldsymbol{\epsilon}\cdot\boldsymbol{\sigma}/2$ according to (3B.3) and (3B.4):

$$\begin{aligned} R(d\boldsymbol{\alpha}')B(d\boldsymbol{\zeta}') &= e^{\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2}e^{-d\boldsymbol{\epsilon}\cdot\boldsymbol{\sigma}/2}e^{-\boldsymbol{\zeta}\cdot\boldsymbol{\sigma}/2} = B^{-1}(\boldsymbol{\zeta})B(d\boldsymbol{\epsilon})B(\boldsymbol{\zeta}) \\ &= 1 - \frac{1}{4(\gamma+1)}(\gamma+1+\gamma\mathbf{v}\cdot\boldsymbol{\sigma}))\,\dot{\boldsymbol{\epsilon}}\cdot\boldsymbol{\sigma}\frac{1}{\sqrt{2(\gamma+1)}}(\gamma+1-\gamma\mathbf{v}\cdot\boldsymbol{\sigma}))dt \end{aligned} \tag{3B.17}$$

We now use the rules

$$[\mathbf{a}\cdot\boldsymbol{\sigma},\,\mathbf{b}\cdot\boldsymbol{\sigma}] = 2i\,(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma},\quad \mathbf{a}\cdot\boldsymbol{\sigma}\,\mathbf{b}\cdot\boldsymbol{\sigma}\,\mathbf{c}\cdot\boldsymbol{\sigma} = \mathbf{a}\cdot\mathbf{b}\,\mathbf{c}\cdot\boldsymbol{\sigma} - \mathbf{a}\cdot\mathbf{c}\,\mathbf{b}\cdot\boldsymbol{\sigma} + \mathbf{b}\cdot\mathbf{c}\,\mathbf{a}\cdot\boldsymbol{\sigma} + i\,(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}, \tag{3B.18}$$

to calculate

$$R(d\boldsymbol{\alpha}')B(d\boldsymbol{\zeta}') - 1 = -\frac{dt}{4(\gamma+1)}\left\{\left[(\gamma+1)^2 + v^2\gamma^2\right]\dot{\boldsymbol{\epsilon}}\cdot\boldsymbol{\sigma} - 2\gamma^2\mathbf{v}\cdot\dot{\boldsymbol{\epsilon}}\,\mathbf{v}\cdot\boldsymbol{\sigma} + 2i\gamma\,(\mathbf{v}\times\dot{\boldsymbol{\epsilon}})\cdot\boldsymbol{\sigma}\right\} \tag{3B.19}$$

Expressing v^2 via (3B.10), the bracket simplifies to $2\gamma(\gamma+1)$. After separating $\dot{\boldsymbol{\epsilon}}$ into parallel and orthogonal projections with respect to $\mathbf{v}$, we obtain:

$$R(d\boldsymbol{\alpha}')B(d\boldsymbol{\zeta}') - 1 = -\frac{1}{2}\left[\gamma\dot{\boldsymbol{\epsilon}}_{\|}\cdot\boldsymbol{\sigma} + \dot{\boldsymbol{\epsilon}}_{\perp}\cdot\boldsymbol{\sigma} + \frac{i\gamma}{\gamma+1}(\mathbf{v}\times\dot{\boldsymbol{\epsilon}}_{\perp})\cdot\boldsymbol{\sigma}\right]dt. \tag{3B.20}$$

Comparison with purelor we identify

$$\gamma\mathbf{v}_{\|} = \boldsymbol{\epsilon}_{\|}, \qquad \gamma\mathbf{v}_{\perp} = \boldsymbol{\epsilon}_{\perp}, \tag{3B.21}$$

and find from the remainder

$$R(d\boldsymbol{\alpha}') - 1 = -\frac{i\gamma^2}{(\gamma+1)}(\mathbf{v}\times\dot{\mathbf{v}})\cdot\boldsymbol{\sigma}/2\,dt. \tag{3B.22}$$

This corrsponds to an angular velocity

$$\dot{\boldsymbol{\alpha}}' = \frac{2\gamma^2}{(\gamma+1)}\mathbf{v}\times\dot{\mathbf{v}}. \tag{3B.23}$$

which is has the opposite sign and is twice as big as the first contribution (3B.14). The total angular velocity of Thomas precession is therefore (with proper velocity c factors reinserted):

$$\boldsymbol{\Omega} = \dot{\boldsymbol{\alpha}} + \dot{\boldsymbol{\alpha}}' = \frac{1}{c^2}\frac{\gamma^2}{(\gamma+1)}\mathbf{v}\times\dot{\mathbf{v}}. \tag{3B.24}$$

The above calculations can certainly be also performed in the 4×4-representation of the Lorentz group. As an illustration, let us calculate the analog of (3B.12). We denote the 4×4 -representation $\dot{B}_{\hat{\zeta}}(-\zeta)B_{\hat{\zeta}}(\zeta)$ by $\dot{\Lambda}(-\mathbf{v})\Lambda{-}\mathbf{v})$. Differentiating (3.17) with respect to time we see that

$$\dot{\Lambda}(-\mathbf{v}) = \begin{pmatrix} \dot{\gamma} & -\dot{\gamma}v^i - \gamma\dot{v}^i \\ -\dot{\gamma}v^i - \gamma\dot{v}^i & \dot{\gamma}\dfrac{\gamma(\gamma+2)}{(\gamma+1)^2}\dfrac{v^iv^j}{c^2} + \dfrac{\gamma^2}{\gamma+1}\dfrac{\dot{v}^iv^j + v^i\dot{v}^j}{c^2} \end{pmatrix}. \tag{3B.25}$$

Multiplying this with $\Lambda(\mathbf{v})$ from the right yields for the first row of the product $[\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})]^0{}_i$:

$$\left[\dot{\gamma}\gamma(1-v^2){-}\gamma^2\frac{\dot{v}v}{c^2}, \dot{\gamma}\left(\gamma{-}1{-}\frac{\gamma^2}{\gamma+1}\frac{v^2}{c^2}\right)\frac{v^i}{c}{-}\gamma\frac{\dot{v}^i}{c}{-}\frac{\gamma^3}{\gamma+1}\frac{\dot{v}v}{c^2}\frac{v^i}{c}\right] \tag{3B.26}$$

Using again the relations $\dot{v}v/c^2 = \dot{\gamma}/\gamma^3$, and $v^2/c^2 = (\gamma^2-1)/\gamma^2$ from (3B.10), the first entry and the $\dot{\gamma}$-terms in the second entry disappear, and we remain with

$$[\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})]^0{}_i = \left[0, -\gamma\frac{\dot{v}^i}{c} - \frac{\gamma^3}{\gamma+1}\frac{\dot{v}v}{c^2}\frac{v^i}{c}\right]. \tag{3B.27}$$

Introducing the components $\dot{\mathbf{v}}_{\parallel}$ and $\dot{\mathbf{v}}_{\perp}$ of the acceleration parallel and orthogonal to $\mathbf{v}$, such that $\dot{v}v\mathbf{v} = v^2\mathbf{v}_{\parallel} = (\gamma^2-1)\mathbf{v}_{\parallel})/\gamma^2$, this can be written as in terms of the 4×4 -matrices (3.56) (3.58) generating pure Lorentz transformations. Their first rows are $(M_1)^0{}_i = i(0,1,0,0)$, $(M_2)^0{}_i = i(0,0,1,0)$, $(M_3)^0{}_i = i(0,0,0,1)$, such that we can write with the vector notation $\mathbf{M} \equiv (M_1, M_2, M_3)$:

$$[\dot{\Lambda}(-\mathbf{v})\Lambda(\mathbf{v})]^0{}_i = \frac{i}{c}\left(\gamma^2\dot{\mathbf{v}}_{\parallel} + \gamma\dot{\mathbf{v}}_{\perp}\right)\mathbf{M}. \tag{3B.28}$$

By replacing the generators $\mathbf{M}$ by the 2×2 -generators of pure Lorentz transformations $-i\boldsymbol{\sigma}/2$ we obtain

$$\frac{1}{2c}\left(\gamma^2\dot{\mathbf{v}}_{\parallel} + \gamma\dot{\mathbf{v}}_{\perp}\right)\boldsymbol{\sigma}, \tag{3B.29}$$

in agreement with (3B.15) and (3B.13), if we reintroduce the omitted factor $1/c$.

It is instructive to calculate the same result once more with the help of the spin four-vector introduced in Eq. (3.717). To find the precession rate we compare again the spin at the time t, where the velocity is $\mathbf{v}$, with the spin at $t + dt$, where the velocity is $\mathbf{v}(t + dt)$. During this time, the spin four-vector changes from S^μ to $\bar{S}^\mu \equiv S^\mu + \dot{S}^\mu dt$. The initial spin is obtained by bringing the electron to its rest frame via a deboosting Lorentz transformation $B^{-1}(\boldsymbol{\zeta}) \equiv \Lambda^\mu{}_\nu(-\mathbf{v})$. Using Eq. (3.17) and v^2 from (3B.10), we have

$$S_R{}^i = \Lambda^i{}_\mu(-\mathbf{v})S^\mu = -\gamma\frac{v^i}{c}S^0 + S^i + \frac{\gamma^2}{\gamma+1}\frac{v^iv^j}{c^2}S^j. \tag{3B.30}$$

The final spin is obtained by a similar Lorentz transformation with a slightly different velocity $\mathbf{v}(t + dt)$. The result is

$$\begin{aligned} S_R^i + dS_R^i &= \Lambda^i{}_\mu(-\mathbf{v}(t+dt))(S^\mu + \dot{S}^\mu dt) \qquad (3B.31) \\ &= \Lambda^i{}_\mu(-\mathbf{v})S^\mu + [\dot{\Lambda}^i{}_\mu(-\mathbf{v})S^\mu + \Lambda^i{}_\mu(-\mathbf{v})\dot{S}^\mu]dt \end{aligned}$$

Since the change of the spin four-vector $\dot{S}^\mu$ points in the direction of $u^\mu = (\gamma, \gamma v^i)$ due to Eq. (3.734), and since $\Lambda^i{}_\mu(-\mathbf{v})u^\mu = 0$ [as can easily be seen by substituting u^μ for S^μ in (3B.30)], we obtain

$$\begin{aligned} \dot{S}^i_R &= \frac{dS^i_R}{dt} = \dot{\Lambda}_\mu{}^i(-\mathbf{v})S^\mu \\ &= -\left(\dot{\gamma}\frac{v^i}{c} + \gamma\frac{\dot{v}^i}{c}\right)S^0 + \dot{\gamma}\frac{\gamma(\gamma+2)}{(\gamma+1)^2}\frac{v^iv^j}{c^2}S^j + \frac{\gamma^2}{\gamma+1}\frac{\dot{v}^iv^j + v^i\dot{v}^j}{c^2}S^j. \end{aligned} \tag{3B.32}$$

Expressing S^i with the help of (3.729), and using $\dot{v}v/c^2 = \dot{\gamma}/\gamma^3$, the last term becomes

$$\frac{\gamma^2}{\gamma+1}\frac{v^i\dot{v}^j}{c^2}S^j = \frac{\gamma^2}{\gamma+1}\left(\frac{v^i\dot{v}^j}{c^2}S^j_R + \frac{\gamma^2}{\gamma+1}\frac{v\dot{v}}{c^2}\frac{v^iv^j}{c^2}S^j_R\right) = \frac{\gamma^2}{\gamma+1}\frac{v^i\dot{v}^j}{c^2}S^j_R + \dot{\gamma}\frac{\gamma}{(\gamma+1)^2}\frac{v^iv^j}{c^2}S^j_R.$$

We now use (3.729) and (3.730), to substitute $v^iS^i/c = \gamma v^iS^i_R/c$ and $S^0 = v^iS^i/c = \gamma v^iS^i_R/c$. Then all terms containing $\dot{\gamma}$ cancel each other and we arrive at the formula for the temporal change of the spin vector:

$$\dot{S}^i_R = \frac{1}{c^2}\frac{\gamma^2}{\gamma+1}(v^i\dot{v}^j - \dot{v}^iv^j)S^j_R = -\frac{1}{c^2}\frac{\gamma^2}{\gamma+1}\left[(\mathbf{v}\times\dot{\mathbf{v}})\times\mathbf{S}_R\right]^i \equiv \Omega\times\mathbf{S}_R, \tag{3B.33}$$

with the vector of angular velocity (3B.24). As a rate of change of a three-vector, it corresponds to a pure rotation. With the help of the generators $(L_i)_{jk} = -i\epsilon_{ijk}$ of the rotation group, we may also write

$$\dot{\mathbf{S}}_R = -i(\boldsymbol{\Omega}\cdot\mathbf{L})\mathbf{S}_R. \tag{3B.34}$$

Such kinematic calculations can, incidentally, be done quite elegantly in a geometric approach. One may exploit the fact that the four-velocities $u^\mu \equiv p^\mu/M$ can be written as

$$u^\mu = c(\cosh\zeta, \hat{\boldsymbol{\zeta}}\sinh\zeta), \tag{3B.35}$$

which shows that up to a factor c they are vectors on a unit hyperbola. These are hyperbolic analogs of euclidean vectors

$$u^\mu_E = c(\cos\alpha, \hat{\boldsymbol{\alpha}}\sin\alpha) \tag{3B.36}$$

on a unit sphere. As such, relative rapidities follow the hyperbolic version of spherical trigonometry, called *Lobatschewski Geometry*. The product of three pure Lorentz transformations $B(\boldsymbol{\zeta}) = e^{-\boldsymbol{\zeta}\sigma/2}$ with rapidities $\boldsymbol{\zeta}_a, \boldsymbol{\zeta}_b, \boldsymbol{\zeta}_c$ can be represented as a triangle in hyperbolic space. The angles of the triangle $\gamma_a, \gamma_b, \gamma_c$ indicate the relative angles between the corresponding $\boldsymbol{\zeta}$ vectors, i.e., $\cos\gamma_a = \hat{\boldsymbol{\zeta}}_b\cdot\hat{\boldsymbol{\zeta}}_c$, etc. (see Fig. 3.4). The angles and sides of the triangle are then related by the cosine and sine theorems

$$\cosh\zeta_a = \cosh\zeta_b\cosh\zeta_c - \sinh\zeta_a\sinh\zeta_b\cos\gamma_c, \tag{3B.37}$$

$$\cos\gamma_a = -\cos\gamma_b\cos\gamma_c + \sin\gamma_a\sin\gamma_b\cosh\zeta_c, \tag{3B.38}$$

(3B.39)

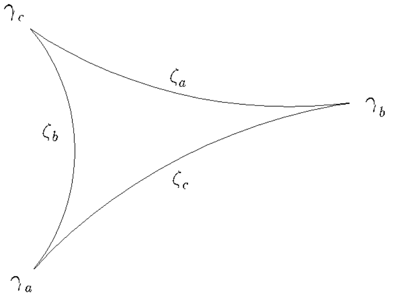

FIGURE 3.4 Triangle formed by rapidities in a hyperbolic space. The sum of angles is smaller than 180^0. The angular defect yields the angle of Thomas precession.

and

$$\frac{\sinh\zeta_a}{\sin\gamma_a}=\frac{\sinh\zeta_b}{\sin\gamma_b}=\frac{\sinh\zeta_c}{\sin\gamma_c}, \tag{3B.40}$$

respectively.

Given two sides and the enclosed angle, say $\zeta_a, \zeta_b, \gamma_c$, we can use *Napier's analogies*

$$\begin{aligned}\frac{\sinh\frac{1}{2}(\zeta_a-\zeta_b)}{\sin\frac{1}{2}(\zeta_a+\zeta_b)} &= \frac{\tan\frac{1}{2}(\gamma_a-\gamma_b)}{\cot\frac{1}{2}\gamma_c}\\ \frac{\cosh\frac{1}{2}(\zeta_a-\zeta_b)}{\cosh\frac{1}{2}(\zeta_a+\zeta_b)} &= \frac{\tan\frac{1}{2}(\gamma_a+\gamma_b)}{\cot\frac{1}{2}\gamma_c}\end{aligned} \tag{3B.41}$$

to calculate the other two angles γ_a, γ_b. After that, either of the two analogous formulas

$$\begin{aligned}\frac{\sin\frac{1}{2}(\gamma_a-\gamma_b)}{\sin\frac{1}{2}(\gamma_b+\gamma_b)} &= \frac{\tanh\frac{1}{2}(\zeta_a-\zeta_b)}{\tanh\frac{1}{2}\zeta_c}\\ \frac{\cos\frac{1}{2}(\gamma_a-\gamma_b)}{\cos\frac{1}{2}(\gamma_a+\gamma_b)} &= \frac{\tanh\frac{1}{2}(\zeta_a+\zeta_b)}{\tanh\frac{1}{2}\zeta_c}\end{aligned} \tag{3B.42}$$

serves to calculate the third side ζ_c.

Since the hyperboloid has a negative unit radius, the sum of the angles is less than π. The angular defect

$$\delta=\pi-\gamma_a-\gamma_b-\gamma_c \tag{3B.43}$$

determines the area A of the triangle. For a hyperbola of radius R:

$$A=R^2E. \tag{3B.44}$$

The angular defect is given in terms of the three sides by the hyperbolic version of the L'Huillier's formula in spherical trigonometry:[26]

$$\tan\frac{1}{4}E=\sqrt{\tanh\frac{s}{2}\tanh\frac{1}{2}(s-\zeta_a)\tanh\frac{1}{2}(s-\zeta_b)\tanh\frac{1}{2}(s-\zeta_c)}, \tag{3B.45}$$

where

$$2s=\zeta_a+\zeta_b+\zeta_c \tag{3B.46}$$

Another formula is

$$\cos(A/2)=\frac{1+\cosh\zeta_a+\cosh\zeta_b+\cosh\zeta_c}{4\cosh^2(\zeta_a/2)\cosh^2(\zeta_b/2)\cosh^2(\zeta_c/2)}. \tag{3B.47}$$

A pure Lorentz transformation of a particle does not change its spin by definition. Such a transformation is therefore a parallel transport along a side of a triangle. When doing three successive parallel transports around a triangle, a particle which was initially at rest comes again to rest. Its spin, however, changes the direction by the angular defect which is determined by the area integral over the curvature. This, in turn, has the constant value -1. Thus formula (3B.47) determines directly the total angle of Thomas precession.

The reader is encouraged to derive the rate of Thomas precession once more using this geometric calculus.[27]

Appendix 3C Clebsch-Gordan Coefficients

A direct product of irreducible representation states $|s_1,m_1\rangle$ and $|s_2,m_2\rangle$ can be decomposed into a sum of irreducible representation states $|sm\rangle$ with total angular momentum $s=|s_1-s_2|,\cdots,(s_1+s_2)$. This is done with the help of Clebsch-Gordan coefficients. For this we multiply any product state with the *completeness relation* of all irreducible representation states

$$\sum_s\sum_{m=-s}^{s}|s,m\rangle\langle s,m|=1, \tag{3C.1}$$

and obtain

$$|s_1,m_1;s_2,m_2\rangle=\sum_{s=|s_1-s_2|}^{s_1+s_2}\sum_{s,m=-s}^{s}|s,m\rangle\langle s,m|s_1,m_1;s_2,m_2\rangle. \tag{3C.2}$$

The expansion coefficients on the right-hand side are the desired Clebsch-Gordan coefficients.

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[26] See, for example, D. D. Ballow and F. H. Steen, *Plane an Spherical Trigonometry with Tables*, Ginn, New York , 1943

[27] For details see J.A. Smorodinskij, Fortschr. Phys. *13*, 157 (1965); A. Sommerfeld, *Electrodynamics*, Academic, New York, 1949.

The expansion (3C.2) can be inverted by means of a similar completeness relation in the product space

$$\sum_{m_1=-s_1}^{s_1} \sum_{m_2=-s_2}^{s_2} |s_1, m_1; s_2, m_2\rangle\langle s_1, m_1; s_2, m_2| = 1, \qquad (3C.3)$$

yielding the expansion

$$|s, m\rangle = \sum_{m_1=-s_1}^{s_1} \sum_{m_2=-s_2}^{s_2} |s_1, m_1; s_2, m_2\rangle\langle s_1, m_1; s_2, m_2|s, m\rangle. \qquad (3C.4)$$

By subjecting these relations to an arbitrary rotation (3.798), and using (3.800), we find the transformation behavior of the Clebsch-Gordan coefficients:

$$D^s_{m,m'}\langle s, m'|s_1, m_1'; s_2, m_2'\rangle (D^s)^{-1}_{m_1',m_1} (D^s)^{-1}_{m_2',m_2} = \langle s, m|s_1, m_1; s_2, m_2\rangle, \qquad (3C.5)$$

or, because of unitarity of the representation matrices,

$$D^s_{m,m'} (D^s_{m_1,m_1'})^* (D^s_{m_2,m_2'})^* \langle s, m'|s_1, m_1'; s_2, m_2'\rangle = \langle s, m|s_1, m_1; s_2, m_2\rangle, \qquad (3C.6)$$

and since the Clebsch-Gordan coefficients are real following the Condon-Shortley convention we also have

$$(D^s_{m,m'})^* D^s_{m_1,m_1'} D^s_{m_2,m_2'} \langle s, m'|s_1, m_1'; s_2, m_2'\rangle = \langle s, m|s_1, m_1; s_2, m_2\rangle, \qquad (3C.7)$$

The Clebsch-Gordan coefficients are related in a simple way to the more symmetric *Wigner 3j-symbols* by defined as follows:

$$\langle s_3, -m_3|s_1, m_1; s_2, m_2\rangle = (-1)^{s_1-s_2-m_3}(2s_3+1)^{1/2} \begin{pmatrix} s_1 & s_2 & s_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \qquad (3C.8)$$

As a consequence of relation (3.836), this has the invariance property

$$D^s_{m_1,m_1'} D^s_{m_2,m_2'} D^s_{m_3,m_3'} \begin{pmatrix} s_1 & s_2 & s_3 \\ m_1' & m_2' & m_3' \end{pmatrix} = \begin{pmatrix} s_1 & s_2 & s_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \qquad (3C.9)$$

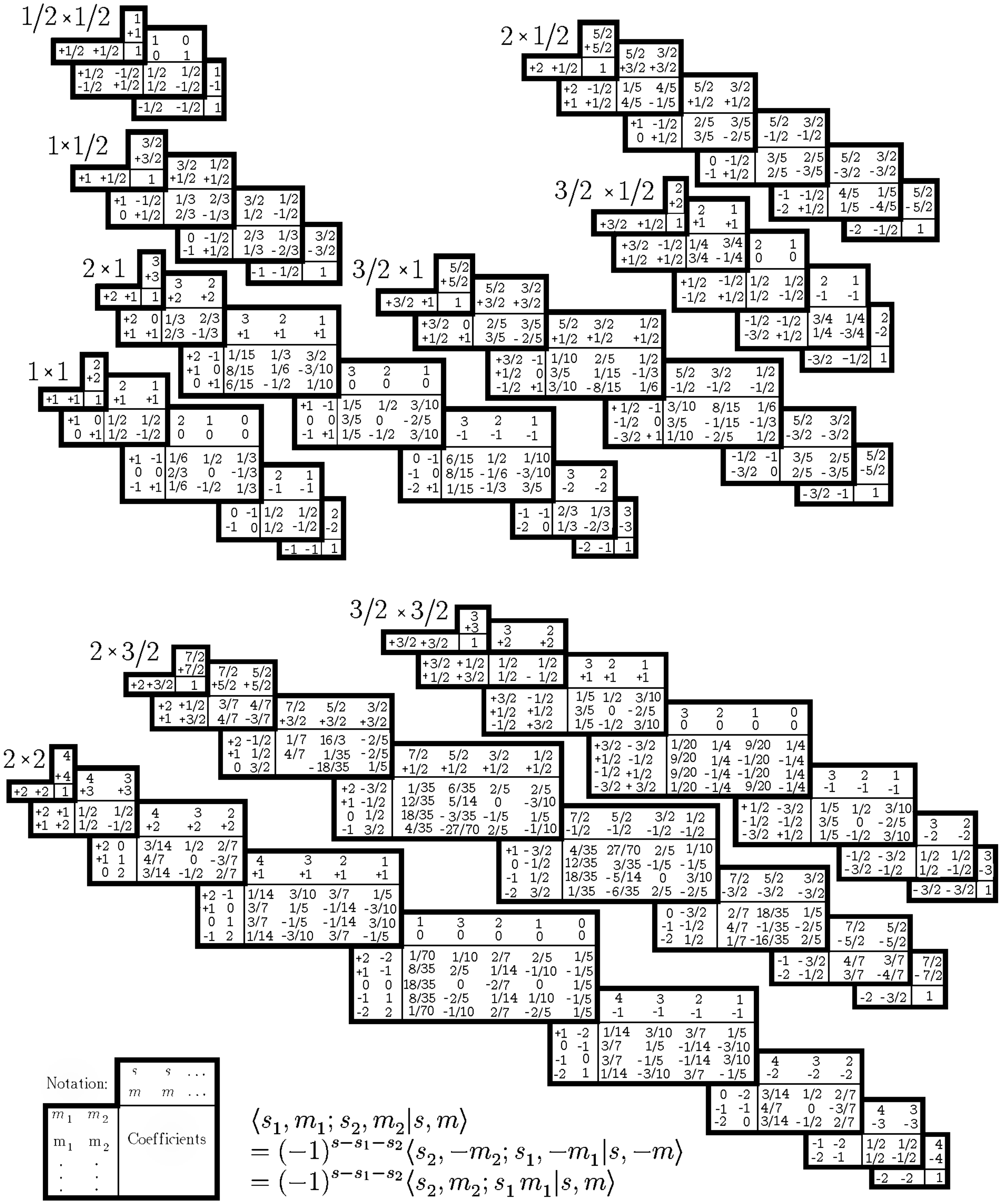
The Levi-Civita symbol ϵ_{ijk} is a cartesian version of the Wigner $3j$-symbol for $s_1 = s_2 = s_3 = 1$. It exhibits the invariance (3C.9) with respect to the 3×3 defining representation matrices of the rotation group:

$$R_{i_1i_1'} R_{i_2i_2'} R_{i_3i_3'} \epsilon_{i_1'i_2'i_3'} = \epsilon_{i_1i_2i_3}. \qquad (3C.10)$$

Under even permutations of columns, the $3j$-symbols are invariant while under odd permutations they pick up a phase factor $(-1)^{s_1+s_2+s_3}$. Also:

$$\begin{pmatrix} s_1 & s_2 & s_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{s_1+s_2+s_3} \begin{pmatrix} s_1 & s_2 & s_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \qquad (3C.11)$$

TABLE 3.2 The lowest Clebsch-Gordan coefficients $\langle s,m|s_1,m_1;s_2,m_2\rangle$. The table entries ±CG are to be read as $\pm\sqrt{\text{CG}}$. The coefficients are all real, i.e. equal to $\langle s_1,m_1;s_2,m_2|s,m\rangle$. For more symmetry properties see Eqs. (3C.22).


1/2×1/2
1×1/2
2×1
1×1
3/2×1
2×1/2
3/2×1/2
3/2×3/2
2×3/2
2×2
Notation:
Coefficients

$$\langle s_1,m_1;s_2,m_2|s,m\rangle = (-1)^{s-s_1-s_2}\langle s_2,-m_2;s_1,-m_1|s,-m\rangle = (-1)^{s-s_1-s_2}\langle s_2,m_2;s_1\,m_1|s,m\rangle$$

In Eq. (3.841) we introduced a contravariant notation for spin-j objects. This is also done in relation (3C.12), writing it as

$$\langle s_3, m_3 | s_1, m_1; s_2, m_2 \rangle \equiv (-1)^{s_1-s_2-s_3}(2s_3+1)^{1/2} \begin{pmatrix} s_1 & s_2 & m_3 \\ m_1 & m_2 & s_3 \end{pmatrix}. \tag{3C.12}$$

The simplest $3j$-symbol is

$$\begin{pmatrix} j & j & 0 \\ m & m' & 0 \end{pmatrix} = (-1)^{j-m}(2j+1)^{-1/2}\delta_{m,-m'} \tag{3C.13}$$

this being also equal to $(-1)^{2j}c^{(j)}_{m,m'}$. In the contravartiant notation, one has

$$\begin{pmatrix} j & m' & 0 \\ m & j & 0 \end{pmatrix} = (-1)^{2j}(2j+1)^{-1/2}\delta_m{}^{m'}. \tag{3C.14}$$

In order to calculate the Clebsch-Gordan coefficients we observe that the state of maximal quantum numbers $|s_1, s_1; s_2, s_2\rangle$ is a state $|s, m\rangle$ of the irreducible representation with the maximal angular momentum $s = m = s_1 + s_2$. By repeatedly applying the lowering operator of angular momentum to it according to the general relation (3.784), we obtain the matrix elements (compare Fig. 3.3)

$$\begin{aligned} L_-|s,s\rangle &= \sqrt{(2s)\cdot 1}|s,s-1\rangle, \\ L_-|s,s-1\rangle &= \sqrt{(2s-1)\cdot 2}|s,s-1\rangle, \\ &\vdots \\ L_-|s,-s+2\rangle &= \sqrt{(2s-1)\cdot 2}|s,-s+1\rangle, \\ L_-|s,-s+1\rangle &= \sqrt{(2s)\cdot 1}|s,-s\rangle. \end{aligned} \tag{3C.15}$$

In the direct-product space, an application of the lowering operator $L_- \times 1 + 1 \times L_-$ to the state $|s_1, s_1; s_2, s_2\rangle$ yields, with the same rules as in (3C.15),

$$\begin{aligned} (L_- \times 1 + 1 \times L_-)|s_1, s_1; s_2, s_2\rangle &= \sqrt{(2s_1)\cdot 1}|s_1, s_1-1; s_2, s_2\rangle \\ &+ \sqrt{(2s_2)\cdot 1}|s_1, s_1; s_2, s_2-1\rangle. \end{aligned} \tag{3C.16}$$

Continuing this with the help of the general relation

$$\begin{aligned} (L_- \times 1 + 1 \times L_-)|s_1, m_1; s_2, m_2\rangle &= \sqrt{(s_1+m_1)(s_1-m_1+1)}|s_1, m_1-1; s_2, m_2\rangle \\ &+ \sqrt{(s_2+m_2)(s_2-m_2+1)}|s_1, m_1; s_2, m_2-1\rangle, \end{aligned} \tag{3C.17}$$

we find all other states $|s, m\rangle$ of the irreducible representation with $s = s_1 + s_2$.

The state of the lower total angular momentum s_1+s_2-1 with maximal magnetic quantum number $m=s$ is obtained from the orthogonal combination of (3C.17):

$$|s_1+s_2-1,s_1+s_2-1\rangle=\sqrt{(2s_1)\cdot 1}|s_1,s_1-1;s_2,s_2\rangle-\sqrt{(2s_2)\cdot 1}|s_1s_1;s_2s_2-1\rangle. \tag{3C.18}$$

This can be verified by applying to it the raising operator $(L_+\times 1+1\times L_+)$: generalizing (3.784) to the direct-product space:

$$\begin{aligned}(L_+\times 1+1\times L_+)|s_1,m_1;s_2,m_2\rangle &= \sqrt{(s_1-m_1)(s_1+m_1+1)}|s_1,m_1+1;s_2,m_2\rangle\\ &+ \sqrt{(s_2-m_2)(s_2+m_2+1)}|s_1,m_1;s_2,m_2+1\rangle,\end{aligned} \tag{3C.19}$$

and finding that it is annihilated.

By applying the lowering operator to the state (3C.18). we generate all states of the irreducible representation $|s_1+s_2-1,m\rangle$ with $m=-s_1-s_2+1,\dots,s_1+s_2-1$.

Multiplying (3C.17) from the left by $\langle s,m|$ and using the hermitian adjoint of relation (3.784), we obtain the recursion relation

$$\begin{aligned}&\sqrt{(s+m)(s-m+1)}\langle s_1,m_1;s_2,m_2|s,m\rangle\\ &\qquad=\sqrt{(s_1-m_1+1)(s_1+m_1)}\langle s_1,m_1-1;s_2,m_2|s,m-1\rangle\\ &\qquad+\sqrt{(s_2-m_2+1)(s_2+m_2)}\langle s_1,m_1;s_2,m_2-1|s,m-1\rangle.\end{aligned} \tag{3C.20}$$

Similarly we can multiply the raising operator relation (3C.19) in the direct-product space multiply it by $\langle s,m|$ from the left and the adjoint of (3.783) to find

$$\begin{aligned}&\sqrt{(s-m)(s+m+1)}\langle s_1,m_1;s_2,m_2|s,m\rangle\\ &\qquad=\sqrt{(s_1+m_1+1)(s_1-m_1)}\langle s_1,m_1+1;s_2,m_2|s,m+1\rangle\\ &\qquad+\sqrt{(s_2+m_2+1)(s_2-m_2)}\langle s_1,m_1;s_2,m_2+1|s,m+1\rangle.\end{aligned} \tag{3C.21}$$

The Clebsch-Gordan coefficients have the following important symmetry properties:

$$\begin{aligned}\langle s,m|s_1,m_1;s_2,m_2\rangle &= (-1)^{j-s_1-s_2}\langle s,m|s_2,m_2;s_1,m_1\rangle\\ &= \langle s,-m|s_2,-m_2;s_1,-m_1\rangle\\ &= (-1)^{j-s_1-s_2}\langle s,-m|s_1,-m_1;s_2,-m_2\rangle\\ &= (-1)^{s_1-m_1}\sqrt{\frac{2s+1}{2s_2+1}}\langle s_2,-m_2|s_1,m_1;s,-m\rangle\\ &= (-1)^{s_2+m_2}\sqrt{\frac{2s+1}{2s_1+1}}\langle s_1,-m_1|s,-m;,s_2,-m_3\rangle.\end{aligned} \tag{3C.22}$$

Some frequently-needed values are listed in Table 3.2.

Appendix 3D Spherical Harmonics

The spherical harmonics are defined as

$$Y_{lm}(\theta,\varphi) \equiv (-1)^m \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\varphi}, \tag{3D.1}$$

where $P_l^m(z)$ are the *associated Legendre polynomials*

$$P_l^m(z) = \frac{1}{2^l l!}(1-z^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(z^2-1)^l. \tag{3D.2}$$

The spherical harmonics are orthonormal with respect to the rotation-invariant scalar product

$$\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi \; Y_{lm}^*(\theta,\varphi)Y_{l'm'}(\theta,\varphi) = \delta_{ll'}\delta_{mm'}. \tag{3D.3}$$

Explicitly, they read for the lowest few angular momenta:

$$\begin{aligned}
Y_{0,0}(\theta,\phi) &= \frac{1}{2\sqrt{\pi}}, \\
Y_{11}(\theta,\phi) &= -\sqrt{\frac{3}{4\pi}}\sin\theta\frac{1}{\sqrt{2}}e^{i\phi}, \\
Y_{10}(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta, \\
Y_{22}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\phi}, \\
Y_{21}(\theta,\phi) &= -\sqrt{\frac{15}{8\pi}}\sin\theta\,\cos\theta\, e^{i\phi}, \\
Y_{20}(\theta,\phi) &= \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right), \\
Y_{33}(\theta,\phi) &= -\frac{1}{4}\sqrt{\frac{35}{4\pi}}\sin^3\theta\, e^{3i\phi}, \\
Y_{32}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\,\cos\theta\, e^{2i\phi}, \\
Y_{31}(\theta,\phi) &= -\frac{1}{4}\sqrt{\frac{21}{4\pi}}\sin\theta\left(5\cos^2\theta - 1\right)e^{i\phi}, \\
Y_{30}(\theta,\phi) &= \sqrt{\frac{7}{4\pi}}\left(\frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta\right).
\end{aligned} \tag{3D.4}$$

The spherical harmonics with negative magnetic quantum number m are obtained via the relation

$$Y_{lm}(\theta,\phi) = (-1)^m Y^*_{l,-m}(\theta,-\phi). \tag{3D.5}$$

For $m=0$, the spherical harmonics reduce to

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta), \tag{3D.6}$$

where

$$P_l(z) \equiv P_l^0(z) = \frac{1}{2^l l!}\frac{d^l}{dz^l}(z^2-1)^l \tag{3D.7}$$

are the *Legendre polynomials.*

For integer $j=l$, the rotation functions $d^j_{m,m'}(\beta)$ can be derived recursively from $d^l_{m,0}(\beta) = P_l(\cos\theta)$ with the help of the recursion relation

$$\begin{aligned}2\sqrt{(j+m')(j+m'-1)}d^j_{m,m'}(\beta) &= \sqrt{(j+m)(j+m-1)}(1+\cos\theta)\,d^{j-1}_{m-1,m'-1}(\beta)\\ &+2\sqrt{j^2-m^2}\sin\theta\,d^{j-1}_{m,m'-1}(\beta) + \sqrt{(j-m)(j-m-1)}(1-\cos\theta)\,d^{j-1}_{m+1,m'-1}(\beta).\end{aligned} \tag{3D.8}$$

For an iterative determination of the rotation functions $d^j_{m,m'}(\beta)$ with half-integer j we use the recursion relation

$$d^j_{m',m}(\beta) = \sqrt{\frac{j-m'}{j-m}}d^{j-1/2}_{m'+1/2,m+1/2}\cos\frac{\beta}{2} + \sqrt{\frac{j+m'}{j-m}}d^{j-1/2}_{m'-1/2,m+1/2}\sin\frac{\beta}{2}. \tag{3D.9}$$

Inserting $m=-1/2$ and using (3.811), we deduce

$$d^j_{m\,1/2}(\beta) = \sqrt{\frac{j+m}{j+1/2}}d^{j-1/2}_{m-1/2,0}\cos\frac{\beta}{2} - \sqrt{\frac{j-m}{j+1/2}}d^{j-1/2}_{m+1/2,0}\sin\frac{\beta}{2}. \tag{3D.10}$$

For $j=l+1/2$, the right-hand side contains only Legendre polynomials. Starting from these $d^j_{m,1/2}(\beta)$, we find all other rotation functions with half-integer j the recursion relation (3D.8).

For $j=1/2$ and $j=1$, the explicit results were given in Eqs. (3.816) and (3.817). For $j=3/2$ we obtain

$$\begin{aligned}d^{3/2}_{3/2,3/2}(\beta) &= \frac{1}{2}(1+\cos\beta)\cos\frac{\beta}{2},\\ d^{3/2}_{3/2,1/2}(\beta) &= -\frac{\sqrt{3}}{2}(1+\cos\beta)\sin\frac{\beta}{2},\\ d^{3/2}_{3/2,-1/2}(\beta) &= \frac{\sqrt{3}}{2}(1-\cos\beta)\cos\frac{\beta}{2},\\ d^{3/2}_{3/2,-3/2}(\beta) &= -\frac{1}{2}(1-\cos\beta)\sin\frac{\beta}{2},\\ d^{3/2}_{1/2,1/2}(\beta) &= \frac{1}{2}(3\cos\beta-1)\cos\frac{\beta}{2},\\ d^{3/2}_{1/2,-1/2}(\beta) &= \frac{1}{2}(3\cos\beta+1)\sin\frac{\beta}{2}.\end{aligned} \tag{3D.11}$$

The remaining matrix elements are obtained via relations (3.811). Similarly for $j = 2$:

$$\begin{aligned}
d^2_{2,2}(\beta) &= \frac{1}{4}(1+\cos\beta)^2, \\
d^2_{2,1}(\beta) &= -\frac{1}{2}(1+\cos\beta)\sin\beta, \\
d^2_{2,0}(\beta) &= \frac{\sqrt{6}}{4}\sin^2\beta, \\
d^2_{2,-1}(\beta) &= -\frac{1}{2}(1-\cos\beta)\sin\beta \\
d^2_{2,-2}(\beta) &= \frac{1}{4}(1-\cos\beta)^2, \\
d^2_{1,1}(\beta) &= \frac{1}{2}(1+\cos\beta)(2\cos\beta-1), \\
d^2_{1,0}(\beta) &= -\sqrt{\frac{3}{2}}\sin\beta\cos\beta, \\
d^2_{1,-1}(\beta) &= \frac{1}{2}(1-\cos\beta)(2\cos\beta+1), \\
d^2_{0,0}(\beta) &= \frac{1}{2}(3\cos^2\beta-1).
\end{aligned} \tag{3D.12}$$

Notes and References

A thorough discussion of the rotation group is found in the textbook
A.R. Edmonds, *Angular Momentum in Quantum Mechanics*, Princeton Univ. Press, 1962.

The Rarita-Schwinger action and its generalizations have been investigated in great detail in attempts to understand the pion nucleon scattering amplitude near the first resonance at around 1240 GeV. Among the many references see:
R.D. Peccei, Phys. Rev. **176**, 1812 (1968);
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V. Bernard, U-G. Meissner Phys. Lett. B **309**, 421 (1993), Phys. Rev. C **52** 2185 (1995);
V. Bernard et al., Int. J. Mod. Phys. E **4**, 193 (1995).

Details and many references can be found in the comprehensive review by
G. Höhler, *Elasic and Charge Exchange Scattering of Elementary Particles*, in Landolt-Börnstein Vol. I/9b2, Springer, Berlin 1983.

4

Relativistic Fields in External Electromagnetic Field

Having found classical fields to describe relativistic particles, we may ask what corrections the relativistic motion causes to the Schrödinger description of atoms. We shall therefore study Klein-Gordon and the Dirac equation in an external field. Let $A_\mu(x)$ be the associated four-vector potential, accounting for electric and magnetic field strengths via (3.222) and (3.223). For classical relativistic point particles, an interaction with these external fields is introduced via the so-called *minimal substitution law*, which we are now going to discuss.

4.1 Minimal Substitution Law and Gauge Invariant Electromagnetic Interaction

The free Lagrangian densities of charged scalar and spin-1/2 particles are from Eqs (3.162) and (3.455):

$$\mathcal{L} = \partial_\mu \phi^*(x) \partial^\mu \phi(x) - M^2 \phi^*(x)\phi(x) \tag{4.1}$$

and

$$\mathcal{L}(x) \;=\; \bar\psi(x)\,(i\not{\partial} - m)\,\psi(x). \tag{4.2}$$

The electromagnetic field is described by the Lagrange density

$$\mathcal{L}(x) \;=\; -\frac{1}{4}F_{\mu\nu}^2(x) = -\frac{1}{4}\left[\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)\right]^2, \tag{4.3}$$

but this will not be of interest in this chapter, since we shall assume a given vector potential from the outset, not worrying about its origin. Only one property of the electromagnetic field will be important in this context: the gauge invariance. In Eqs. (3.225) and (3.226) we have expressed electric and magnetic field strength as components of a four-curl $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ of a vector potential $A_\mu(x)$. This four-curl is invariant under gauge transformations

$$A_\mu(x) \to A_\mu(x) + \partial_\mu \Lambda(x). \tag{4.4}$$

This gauge invariance has to be maintained in introducing electromagnetic interactions into the Lagrange densities (4.1) and (4.2) of charged scalar and Dirac fields. The prescription for finding such a coupling has been known for a long time in the classical electrodynamics of point particles: There, a free relativistic particle moving along an arbitrary parametrized path $x^\mu(\tau)$ in four-space is described by an action

$$\mathcal{A} = -Mc^2 \int d\tau \sqrt{\frac{dx^\mu}{d\tau}\frac{dx_\mu}{d\tau}} = -mc^2 \int dt \left[1 - \frac{\mathbf{v}^2(t)}{c^2}\right]^{1/2}, . \tag{4.5}$$

where $x^0(\tau) = t$ is the time and $d\mathbf{x}/dt = \mathbf{v}(t)$ the velocity along the path. If the particle has a charge e and lies at rest at position $\mathbf{x}$, its potential energy is

$$V(\mathbf{x}, t) = e\phi(\mathbf{x}, t) \tag{4.6}$$

where

$$\phi(\mathbf{x}, t) = A^0(\mathbf{x}, t). \tag{4.7}$$

In our convention, the charge of the electron e has a negative value to have agreement with the sign in the historic form of the Maxwell equations

$$\begin{aligned} \boldsymbol{\nabla} \cdot \mathbf{E}(x) &= -\boldsymbol{\nabla}^2 \phi(x) = \rho(x), \\ \boldsymbol{\nabla} \times \mathbf{B}(x) - \dot{\mathbf{E}}(x) &= \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \mathbf{A}(x) - \dot{\mathbf{E}}(x) \\ &= -\left[\boldsymbol{\nabla}^2 \mathbf{A}(x) - \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \mathbf{A}(x)\right] - \dot{\mathbf{E}}(x) = \frac{1}{c}\mathbf{j}(x). \end{aligned} \tag{4.8}$$

If the electron moves along a trajectory $\mathbf{x}(t)$, the potential energy becomes

$$V(t) = e\phi\left(\mathbf{x}(t), t\right). \tag{4.9}$$

In the Lagrangian $L = T - V$ this contributes with the opposite sign

$$L^{\text{int}}(t) = -eA^0\left(\mathbf{x}(t), t\right) \tag{4.10}$$

giving a potential part of the interaction

$$\mathcal{A}^{\text{int}}\big|_{\text{pot}} = -e \int dt A^0\left(\mathbf{x}(t), t\right). \tag{4.11}$$

Since the time t coincides with $x^0(t)/c$ of the trajectory, this can be expressed as

$$\mathcal{A}^{\text{int}}\big|_{\text{pot}} = -\frac{e}{c} \int dx^0 A^0(x). \tag{4.12}$$

In this form it is now quite simple to write down the complete electromagnetic interaction purely on the basis of relativistic invariance. The minimal invariant extension of (4.13) is obviously

$$\mathcal{A}^{\text{int}} = -\frac{e}{c} \int dx^\mu A_\mu(x). \tag{4.13}$$

Thus, the full action of a point particle can be written more explicitly as

$$\begin{aligned}\mathcal{A} &= \int dt L(t) = -mc\int ds - \frac{e}{c}\int dx^\mu A_\mu(x) \\ &= -mc^2\int dt\left[1-\frac{\mathbf{v}^2}{c^2}\right]^{1/2} - e\int dt\left(A^0 - \frac{1}{c}\mathbf{v}\cdot\mathbf{A}\right).\end{aligned} \tag{4.14}$$

The canonical formalism supplies the canonically conjugate momenta

$$\mathbf{P} = \frac{\partial L}{\partial \mathbf{v}} = m\frac{\mathbf{v}}{\sqrt{1-\mathbf{v}^2/c^2}} + \frac{e}{c}\mathbf{A} \equiv \mathbf{p} + \frac{e}{c}\mathbf{A}. \tag{4.15}$$

Thus the velocity is related to the canonical momenta and external field via

$$\frac{\mathbf{v}}{c} = \frac{\mathbf{P}-\frac{e}{c}\mathbf{A}}{\sqrt{\left(\mathbf{P}-\frac{e}{c}\mathbf{A}\right)^2 + m^2c^2}}. \tag{4.16}$$

This can be used to calculate the Hamiltonian via the Legendre transform

$$H = \frac{\partial L}{\partial \mathbf{v}}\mathbf{v} - L = \mathbf{P}\cdot\mathbf{v} - L \tag{4.17}$$

giving

$$H = c\sqrt{\left(\mathbf{P}-\frac{e}{c}\mathbf{A}\right)^2 + m^2c^2} + eA^0. \tag{4.18}$$

In the non-relativistic limit this has the expansion

$$H = mc^2 + \frac{1}{2m}\left(\mathbf{P}-\frac{e}{c}\mathbf{A}\right)^2 + eA^0 + \dots \tag{4.19}$$

Thus the free theory goes over into the interacting theory by what is called the *minimal substitution* law

$$\begin{aligned}\mathbf{p} &\rightarrow \mathbf{p} - \frac{e}{c}\mathbf{A} \\ H &\rightarrow H - \frac{e}{c}A^0\end{aligned} \tag{4.20}$$

or, in relativistic notation,

$$p^\mu \rightarrow p^\mu - \frac{e}{c}A^\mu. \tag{4.21}$$

When going over from quantum mechanics to second quantized field theories we found the rule that a non-relativistic Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \tag{4.22}$$

became an operator

$$H = \int d^3x \psi^\dagger(\mathbf{x},t) \left[-\frac{\partial_{\mathbf{x}}{}^2}{2m} + V(\mathbf{x}) \right] \psi(\mathbf{x},t), \tag{4.23}$$

where we have omitted the operator hats, for brevity. With the same rules we see that the second quantized form of the interacting nonrelativistic Hamiltonian in a static $A(\mathbf{x})$ field,

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + \frac{e}{c} A^0, \tag{4.24}$$

is given by

$$H = \int d^3x \psi^\dagger(\mathbf{x},t) \left[-\frac{1}{2m} \left(\partial_{\mathbf{x}} - i\frac{e}{c}\mathbf{A} \right)^2 + eA^0(\mathbf{x}) \right] \psi(\mathbf{x},t). \tag{4.25}$$

When going to the action of this theory we find

$$\begin{aligned} \mathcal{A} = \int dt L = \int dt \int d^3x \, \Big[& \psi^\dagger(\mathbf{x},t) \left(i\partial_t + eA^0 \right) \psi(\mathbf{x},t) \\ & + \frac{1}{2m} \psi^\dagger(\mathbf{x},t) \left(\partial_{\mathbf{x}} - i\frac{e}{c}\mathbf{A} \right)^2 \psi(\mathbf{x},t) \Big]. \end{aligned} \tag{4.26}$$

It is easy to verify that (4.25) reemerges from the Legendre transform

$$H = \frac{\partial L}{\partial \dot{\psi}(\mathbf{x},t)} \dot{\psi}(\mathbf{x},t) - L. \tag{4.27}$$

The action (4.26) holds also for time-dependent $A^\mu(x)$ fields.

We can now deduce the second quantized form of the minimal substitution law (4.20) which is

$$\begin{aligned} \partial_{\mathbf{x}} &\to \partial_{\mathbf{x}} - i\frac{e}{c}\mathbf{A}(\mathbf{x},t), \\ \partial_t &\to \partial_t + ieA^0(\mathbf{x},t), \end{aligned} \tag{4.28}$$

or covariantly:

$$\partial_\mu \to \partial_\mu + i\frac{e}{c} A_\mu(x). \tag{4.29}$$

This substitution rule has the important property that the gauge invariance of the free photon action is preserved by the interacting theory: If we perform the gauge transformation

$$A^\mu(x) \to A^\mu(x) + \partial^\mu \Lambda(x), \tag{4.30}$$

i.e.,

$$\begin{aligned} A^0(\mathbf{x},t) &\to A^0(\mathbf{x},t) + \partial_t \Lambda(\mathbf{x},t) \\ \mathbf{A}(\mathbf{x},t) &\to \mathbf{A}(\mathbf{x},t) - \boldsymbol{\nabla}\Lambda(\mathbf{x},t), \end{aligned} \tag{4.31}$$

the action remains invariant if we simultaneously change the fields $\psi(\mathbf{x},t)$ of the charged particles by a spacetime-dependent phase

$$\psi\,(\mathbf{x},t) \to e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\psi(\mathbf{x},t). \tag{4.32}$$

Under this transformation, the derivatives of the field change like

$$\begin{aligned} \partial_{\mathbf{x}}\psi(\mathbf{x},t) &\to e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left[\partial_{\mathbf{x}} - i\frac{e}{c}\partial_{\mathbf{x}}\Lambda(\mathbf{x},t)\right]\psi, \\ \partial_t\psi &\to e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left(\partial_t - ie\partial_t\Lambda\right)\psi(\mathbf{x},t). \end{aligned} \tag{4.33}$$

The modified derivatives appearing in the action have therefore the following simple transformation law:

$$\begin{aligned} \left(\partial_{\mathbf{x}} - i\frac{e}{c}\mathbf{A}\right)\psi(\mathbf{x},t) &\to e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left(\partial_{\mathbf{x}} - i\frac{e}{c}\mathbf{A}\right)\psi(\mathbf{x},t), \\ \left(\partial_t + i\frac{e}{c}A^0\right)\psi(\mathbf{x},t) &\to e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left(\partial_t + ieA^0\right)\psi(\mathbf{x},t). \end{aligned} \tag{4.34}$$

These combinations of derivatives and gauge fields are called *covariant derivatives* and written as

$$\begin{aligned} \mathbf{D}\psi(\mathbf{x},t) &\equiv \left(\partial_{\mathbf{x}} - i\frac{e}{c}\mathbf{A}\right)\psi(\mathbf{x},t) \\ D_t\psi(\mathbf{x},t) &\equiv \left(\partial_t + ieA^0\right)\psi(\mathbf{x},t) \end{aligned} \tag{4.35}$$

or, in four-vector notation,

$$D_\mu\psi(x) = \left(\partial_\mu + i\frac{e}{c}A_\mu\right)\psi(x). \tag{4.36}$$

Here the adjective covariant does not refer to the Lorentz group but to the gauge group. It records the fact that $D_\mu\psi$ transforms under local gauge changes (4.28) of ψ in the same way as ψ itself in (4.32):

$$D_\mu\psi(x) \to e^{-i\frac{e}{c}\Lambda(x)}D_\mu\psi(x). \tag{4.37}$$

With the help of this covariant derivative any action, which is invariant under global phase changes by a constant phase angle

$$\psi(x) \to e^{-i\phi}\psi(x), \tag{4.38}$$

can easily be made invariant under local gauge transformations (4.30). We merely have to replace all derivatives by covariant derivatives (4.36) and adding the gauge invariant photon Lagrangian (4.3).

For a relativistic scalar field of charge e, the interacting Lagrange density is a straightforward generalization of the Schrödinger case (4.26):

$$\begin{aligned} \mathcal{L} &= [D_\mu\phi(x)]^* D^\mu\phi(x) - M^2\phi^*(x)\phi(x) \\ &= \left[\partial_\mu - i\frac{e}{c}A_\mu(x)\right]\phi(x)\left[\partial^\mu + i\frac{e}{c}A^\mu(x)\right]\phi(x) - M^2\phi^*(x)\phi(x) \end{aligned} \tag{4.39}$$

For relativistic spin-1/2 particles of charge e, we replace in the Lagrangian (4.2):

$$\not\partial = \gamma^\mu \partial_\mu \rightarrow \gamma^\mu \left(\partial_\mu + i\frac{e}{c}A_\mu\right) = \left(\not\partial + i\frac{e}{c}\not A\right) \equiv \not D\,. \tag{4.40}$$

In this way we arrive at the Lagrangian of quantum electrodynamics (QED)

$$\mathcal{L}(x) = \bar\psi(x)\,(i\not D - m)\,\psi(x) - \frac{1}{4}F_{\mu\nu}^2. \tag{4.41}$$

The classical field equations can easily be found by extremizing the action and variation with respect to all fields which gives

$$\frac{\delta\mathcal{A}}{\delta\bar\psi(x)} = (i\not D - M)\,\psi(x) = 0 \tag{4.42}$$

$$\frac{\delta\mathcal{A}}{\delta A_\mu(x)} = \partial_\nu F^{\nu\mu}(x) - \frac{1}{c}j^\mu(x) = 0. \tag{4.43}$$

with the *current density*

$$j^\mu(x) \equiv e\,c\,\bar\psi(x)\gamma^\mu\psi(x). \tag{4.44}$$

Equation (4.43) coincides Maxwell equation for the electromagnetic field around a classical four-dimensional vector current $j^\mu(x)$:

$$\partial_\nu F^{\nu\mu}(x) = \frac{1}{c}j^\mu(x). \tag{4.45}$$

In the Lorentz gauge $\partial_\mu A^\mu(x) = 0$, this equation reads simply

$$-\,\partial^2 A^\mu(x) = \frac{1}{c}j^\mu(x). \tag{4.46}$$

The current j^μ combines the charge density $\rho(x)$ and the current density $\mathbf{j}$ of particles of charge e in a four-vector

$$j^\mu = (c\rho, \mathbf{j})\,. \tag{4.47}$$

In terms of electric and magnetic fields $E^i = F^{i0}$, $B^i = -F^{jk}$, the field equations (4.45) turn into the Maxwell equations

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{E} &= \rho = e\bar\psi\gamma^0\psi = e\psi^\dagger\psi \\ \boldsymbol{\nabla}\times\mathbf{B} - \dot{\mathbf{E}} &= \frac{1}{c}\mathbf{j} = \frac{e}{c}\bar\psi\boldsymbol{\gamma}\psi. \end{aligned} \tag{4.48}$$

The first is Coulomb's law, the second Ampere's law in the presence of charges and currents.

Note that the physical units employed here differ from those used in many books of classical electrodynamics[1] by the absence of a factor $1/4\pi$ on the right-hand side. The Lagrangian used in those books is

$$\begin{aligned} \mathcal{L}(x) &= -\frac{1}{8\pi}F_{\mu\nu}^2(x) - \frac{1}{c}j^\mu(x)A_\mu(x) \\ &= \frac{1}{4\pi}\left[\mathbf{E}^2 - \mathbf{B}^2\right](x) - \left[\rho\phi - \frac{1}{c}\mathbf{j}\cdot\mathbf{A}\right](x), \end{aligned} \tag{4.49}$$

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[1] See for example J. D. Jackson, *Classical Electrodynamics*, Wiley and Sons, New York, 1967.

which leads to Maxwell's field equations

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{E} &= 4\pi\rho \\ \boldsymbol{\nabla}\times\mathbf{B} &= \frac{4\pi}{c}\mathbf{j}. \end{aligned} \tag{4.50}$$

The form employed conventionally in quantum field theory arises from this by replacing $A \longrightarrow \sqrt{4\pi}A$ and $e \longrightarrow \sqrt{4\pi}e$. The charge of the electron in our units has therefore the numerical value

$$e = -\sqrt{4\pi\alpha} \approx -\sqrt{4\pi/137} \tag{4.51}$$

rather than $e = -\sqrt{\alpha}$.

4.2 Pauli Equation

It is instructive to take the Dirac equation (4.42) to a two-component form corresponding to (3.519) and (3.520), and further to (3.526). Due to the fundamental nature of the equations to be derived we shall not work with natural units in this section but carry all fundamental constants along explicitly. As in (3.527), we multiply (4.42) by $(i\hbar\not{D} - Mc)$ and work out the product

$$(i\hbar\not{D} - Mc)\,(i\hbar\not{D} + Mc) = \left[i\gamma^\mu\left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right) + Mc\right]\left[i\gamma^\mu\left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right) - Mc\right] \tag{4.52}$$

We now use the relation

$$\gamma^\mu\gamma^\nu = \frac{1}{2}(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu) + \frac{1}{2}(\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu) = g^{\mu\nu} - i\sigma^{\mu\nu}, \tag{4.53}$$

with $\sigma^{\mu\nu}$ from (3.471), and find

$$\begin{aligned} &\gamma^\mu\gamma^\nu\left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right)\left(\partial_\mu + i\frac{e}{c}A_\mu\right) \\ &\quad = g^{\mu\nu}\left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right)\left(\partial_\mu + i\frac{e}{c}A_\mu\right) - \frac{i}{2}\sigma^{\mu\nu}[\hbar\partial_\mu + i\frac{e}{c}A_\mu, \hbar\partial_\nu + i\frac{e}{c}A_\nu] \\ &\quad = \left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right)^2 + \frac{1}{2}\frac{e\hbar}{c}\sigma^{\mu\nu}F_{\mu\nu}. \end{aligned} \tag{4.54}$$

Thus we obtain as a generalization of Eqs. (3.526) the *Pauli equation*

$$\left[-\left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right)^2 - \frac{1}{2}\frac{e\hbar}{c}\sigma^{\mu\nu}F_{\mu\nu} - M^2c^2\right]\psi(x) = 0, \tag{4.55}$$

and the same equation once more for the other two-component spinor field $\eta(x)$. The spin is coupled to the electromagnetic field strengths via the term

$$\frac{1}{2}\sigma^{\mu\nu}F_{\mu\nu} = -\boldsymbol{\Sigma}\cdot\mathbf{H} + i\boldsymbol{\alpha}\cdot\mathbf{E}. \tag{4.56}$$

where in the chiral and Dirac representations

$$\boldsymbol{\alpha} = \begin{pmatrix} -\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \qquad \boldsymbol{\alpha}_{\rm D} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \tag{4.57}$$

respectively. Thus, in the chiral representation, Eq. (4.55) decomposes into two separate two-component equations for the upper and lower spinor components $\xi(x)$ and $\eta(x)$ in $\psi(x)$:

$$\left[-\left(\hbar\partial_\mu + i\frac{e}{c}A_\mu\right)^2 + \boldsymbol{\sigma}\cdot(\mathbf{H}\pm i\mathbf{E}) - M^2c^2\right]\left\{\begin{matrix}\xi(x)\\ \eta(x)\end{matrix}\right\} = 0. \tag{4.58}$$

In the nonrelativistic limit where $c \to \infty$, we remove the fast oscillations from $\xi(x)$, setting $\xi(x) \equiv e^{-iMc^2t/\hbar}\Psi(\mathbf{x},t)/\sqrt{2M}$ as in (3.151), and find for $\Psi(\mathbf{x},t)$ the nonrelativistic equation

$$\left[i\partial_t + \frac{\hbar^2}{2M}\left(\boldsymbol{\nabla} - i\frac{e}{c\hbar}\mathbf{A}\right)^2 + \frac{e}{2Mc}\boldsymbol{\sigma}\cdot\mathbf{H} - eA^0(x)\right]\Psi(\mathbf{x},t) = 0. \tag{4.59}$$

This corresponds to a magnetic interaction energy

$$H_{\rm mag} = -\frac{e\hbar}{2Mc}\boldsymbol{\sigma}\cdot\mathbf{H}. \tag{4.60}$$

For a small magnet with a magnetic moment $\boldsymbol{\mu}$, the magnetic interaction energy is

$$H_{\rm mag} = -\boldsymbol{\mu}\cdot\mathbf{H}. \tag{4.61}$$

A Dirac particle with has therefore a magnetic moment

$$\boldsymbol{\mu} = \frac{e}{Mc}\frac{\hbar\boldsymbol{\sigma}}{2} = 2\frac{e}{2Mc}\mathbf{S}, \tag{4.62}$$

where $\mathbf{S} = \boldsymbol{\sigma}/2$ is the spin matrix. Experimentally, one parametrizes a magnetic moment of a fundamental particles as

$$\boldsymbol{\mu} = g\frac{e}{2Mc}\mathbf{S} \tag{4.63}$$

and calls the quantity g is called the *gyromagnetic ratio*. This parametrization is such that a uniformly charged sphere has a gyromagnetic ratio 1. According to the Dirac theory, an electron has a gyromagnetic ratio

$$g_e|_{\rm Dirac} = 2. \tag{4.64}$$

Experimentally, the value is very close to this. The small deviation called anomalous magnetic moments will be explained in Chapter 10.

The nonrelativistic Pauli equation (4.59) could laso have been obtained by introducing a minimal coupling directly into the nonrelativistic two-component equation (3.523). This changes $i\partial_t \to i\partial_t - eA^0$ and $(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})^2 \to [\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla} - ie\mathbf{A})]^2$. The latter is worked out as in (4.65), yielding

$$\begin{aligned}[\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla} - ie\mathbf{A})]^2 &= \left[\delta^{ij} + i\epsilon_{ijk}\sigma^k\right](\nabla_i - ieA_i)(\nabla_j - ieA_j) \\ &= (\boldsymbol{\nabla} - ie\mathbf{A})^2 + i\epsilon_{ijk}\sigma^k(\nabla_i - ieA_i)(\nabla_j - ieA_j) + e\boldsymbol{\sigma}\cdot\mathbf{H}, \end{aligned} \tag{4.65}$$

so that Eq. (3.525) goes over into (4.59), after reinserting all fundamental constants,

4.3 Relativistic Wave Equations in Coulomb Potential

It is now easy to write down field equations for a Klein-Gordon and a Dirac field in the presence of an external Coulomb potential of charge Ze. In natural units we have

$$V_{\rm C}(\mathbf{x}) = -\frac{Z\alpha}{r}, \qquad r = \sqrt{\mathbf{x}^2}, \tag{4.66}$$

corresponding to a four-vector potential

$$eA_\mu(x) = (V_{\rm C}(\mathbf{x},0), \mathbf{0}). \tag{4.67}$$

Since this does not depend on time, we can consider the wave equations for wave functions $\phi(x) = e^{-iEt}\phi_E(\mathbf{x})$ and $\psi(x) = e^{-iEt}\psi_E(\mathbf{x})$, and find the time-independent equations

$$(E^2 + \boldsymbol{\nabla}^2 - M)\phi_E(\mathbf{x}) = 0 \tag{4.68}$$

and

$$(\gamma^0 E + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} - M)\psi_E(\mathbf{x}) = 0. \tag{4.69}$$

In these equations we simply perform the minimal substitution

$$E \to E + \frac{Z\alpha}{r}. \tag{4.70}$$

The energy-eigenvalues obtained from the resulting equations can be compared with those of hydrogen-like atoms. The velocity of an electron in the ground state is of the order αZc. Thus for rather high Z, the electron has a relativistic velocity and there must be corrections significant deviations from Schrödinger theory. We shall see that the Dirac equation in an external field reproduces quite well a number of features resulting from the relativistic motion.

4.3.1 Reminder of Schrödinger Equation for Coulomb Potential

The time-independent Schrödinger equation reads

$$\left(-\frac{1}{2M}\boldsymbol{\nabla}^2 - \frac{Z\alpha}{r} - E\right)\psi_E(\mathbf{x}) = 0. \tag{4.71}$$

The Laplacian may be decomposed into radial and angular parts by writing

$$\boldsymbol{\nabla}^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\hat{\mathbf{L}}^2}{r^2}, \tag{4.72}$$

where $\hat{\mathbf{L}} = \mathbf{x}\times\hat{\mathbf{p}}$ are the differential operators for the generators of angular momentum [the spatial part of $L_i = L^{23}$ of (3.91)]. Then (4.71) reads

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{2}{r}\frac{\partial}{\partial r} + \frac{\hat{\mathbf{L}}^2}{r^2} - \frac{2Z\alpha M}{r} - 2ME\right)\psi_E(x) = 0. \tag{4.73}$$

The eigenstates of $\hat{\mathbf{L}}^2$ are the spherical harmonics $Y_{lm}(\theta,\varphi)$, which diagonalize also the third component of $\hat{\mathbf{L}}$, with the eigenvalues

$$\begin{aligned}\hat{\mathbf{L}}^2 Y_{lm}(\theta,\varphi) &= l(l+1)Y_{lm}(\theta,\varphi),\\ \hat{L}_3 Y_{lm}(\theta,\varphi) &= mY_{lm}(\theta,\varphi).\end{aligned} \tag{4.74}$$

The wave functions may be factorized into a radial wave function $R_{nl}(r)$ and a spherical harmonic:

$$\psi_{nlm}(\mathbf{x}) = R_{nl}(r)Y_{lm}(\theta,\varphi). \tag{4.75}$$

Explicitly,

$$\begin{aligned}R_{nl}(r) &= \frac{1}{a_B^{1/2}n}\frac{1}{(2l+1)!}\sqrt{\frac{(n+l)!}{(n-l-1)!}} \qquad (4.76)\\ &\quad\times(2r/na_B)^{l+1}e^{-r/na_B}M(-n+l+1,2l+2,2r/na_B)\\ &= \frac{1}{a_B^{1/2}n}\sqrt{\frac{(n-l-1)!}{(n+l)!}}e^{-r/na_B}(2r/na_B)^{l+1}L_{n-l-1}^{2l+1}(2r/na_B),\end{aligned}$$

where a_B is the Bohr radius, which in natural units $\hbar = c = 1$ is equal to

$$a_B = \frac{1}{ZM\alpha}, \tag{4.77}$$

For a hydrogen atom with $Z = 1$, this is about 1/137 times the Compton wavelength of the electron. The classical velocity of the electron on the lowest Bohr orbit is $v_B = \alpha c$. Thus it is almost nonrelativistic, which is the reason what the Schrödinger equation explains the hydrogen spectrum quite well. The functions $M(a,b,z)$ are confluent hypergeometric functions or Kummer functions, defined by the power series

$$M(a,b,z) \equiv F_{1,1}(a,b,z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)}\frac{z}{z!} + \dots\ . \tag{4.78}$$

For $b = -n$ they are polynomial related to the Laguerre polynomials[2] $L_n^\mu(z)$ by

$$L_n^\mu(z) \equiv \frac{(n+\mu)!}{n!\mu!}M(-n,\mu+1,z), \tag{4.79}$$

The radial wave functions are normalized to

$$\int_0^\infty dr R_{n_r l}(r)R_{n_r' l}(r) = \delta_{n_r n_r'}. \tag{4.80}$$

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[2] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 8.970 (our definition differs from that in L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Pergamon Press, New York, 1965, Eq. (d.13): Our $L_n^\mu = (-)^\mu/(n+\mu)!L_{n+\mu}{}^\mu|_{\text{L.L.}}$).

They have an asymptotic behavior $P_{nl}(r/n)e^{-r/na_B}$, where $P_{nl}(r/n)$ is a polynomial of degree $n_r = n - l - 1$, which defines the radial *quantum number*. The energy eigenvalues depend on are n in the well-known way:

$$E_n = -Z^2 \frac{M\alpha^2}{2n^2}. \tag{4.81}$$

The number $\alpha^2 M/2$ is the Rydberg-constant:

$$\mathrm{Ry} = \frac{\alpha^2 M}{2} \approx \frac{27.21}{2}\mathrm{eV} \approx 3.288 \times 10^{15}\mathrm{Hz}. \tag{4.82}$$

Later in Section ??) we shall need the value of the wave function at the origin. It is non-zero only for s-waves where it is equal to

$$|\psi_{n00}(\mathbf{0})| = \frac{1}{\sqrt{\pi}}\sqrt{\frac{ZM\alpha}{n}}^{3} = \frac{1}{\sqrt{\pi}}\sqrt{\frac{1}{na_B}}^{3}. \tag{4.83}$$

4.3.2 Klein-Gordon Field in Coulomb Potential

After the substitution (4.70) into (4.68), we find the Klein-Gordon equation in the Coulomb potential (4.66):

$$\left[\left(E + \frac{Z\alpha}{r}\right)^2 + \boldsymbol{\nabla}^2 - M^2\right]\phi_E(\mathbf{x}) = 0. \tag{4.84}$$

After inserting the angular decomposition (4.72), this becomes

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{2}{r}\frac{\partial}{\partial r} + \frac{\hat{\mathbf{L}}^2 - Z^2\alpha^2}{r^2} - \frac{2Z\alpha E}{r} - (E^2 - M^2)\right]\phi_E(\mathbf{x}) = 0. \tag{4.85}$$

The solutions of this equation can be obtained from those of the nonrelativistic Schrödinger equation (4.73) by replacing

$$\hat{\mathbf{L}}^2 \longrightarrow \hat{\mathbf{L}}^2 - Z^2\alpha^2, \tag{4.86}$$

$$\alpha \longrightarrow \alpha\frac{E}{M}, \tag{4.87}$$

$$E \longrightarrow \frac{E^2 - M^2}{2M}. \tag{4.88}$$

The replacement (4.86) is done most efficiently by defining the eigenvalues $l(l+1) - Z^2\alpha^2$ of $\hat{\mathbf{L}}^2 - Z^2\alpha^2$ in analogy to those of $\hat{\mathbf{L}}^2$ as $\lambda(\lambda+1)$:

$$l(l+1) - Z^2\alpha^2 \equiv \lambda(\lambda+1). \tag{4.89}$$

Then the quantum number l of the Schrödinger wave functions is simply replaced by $\lambda_l = l - \delta_l$, where

$$\begin{aligned} \delta_l &= l + \frac{1}{2} - \left[\left(l + \frac{1}{2} \right)^2 - Z^2\alpha^2 \right]^{1/2} \\ &= \frac{Z^2\alpha^2}{2l+1} + \mathcal{O}(\alpha^4). \end{aligned} \tag{4.90}$$

The other solution of relation (4.89) with the opposite sign in front of the square root is unphysical since the associated wave functions are too singular at the origin to be normalizable. As before, the radial quantum number n_r which determines the degree of the polynomial $P_{nl}(r/n)$ in the wave functions must be an integer. This is no longer true for the combination of quantum numbers which determines the energy, which is now given by

$$n_r + \lambda + 1 = n_r + l + 1 - \delta_l = n - \delta_l. \tag{4.91}$$

This leads to the equation for the energy eigenvalues

$$\frac{E_{nl}{}^2 - M^2}{2M} = -\frac{Z^2M\alpha^2}{2}\frac{E_{nl}{}^2}{M^2}\frac{1}{(n-\delta_l)^2}, \tag{4.92}$$

with the solution

$$\begin{aligned} E_{nl} &= \frac{M}{\sqrt{1 + Z^2\alpha^2/(n-\delta_l)^2}} \\ &= M\left[1 - \frac{(Z\alpha)^2}{2n^2} + \frac{3}{8}\frac{(Z\alpha)^4}{n^4} - \frac{(Z\alpha)^4}{n^3(2l+1)} + \mathcal{O}(Z^6\alpha^6) \right]. \end{aligned} \tag{4.93}$$

The first two terms correspond to the Schrödinger energies (4.81) (plus rest energy), the next two are relativistic corrections. The first of these breaks the degeneracy between the levels of the same n and different l, generated in the Schrödinger theory by the Lentz-Runge vector [O(4)-invariance].

The correction terms become large for large central charge Z. In particular, the lowest energy and successively the higher ones become complex for central charges $Z > 137/2$. The physical reason for this is that the large potential gradient near the origin can create pairs of particles from the vacuum. This phenomenon can only be properly understood after quantizing the field theory.

As for the free Klein-Gordon field, the energy appears with both signs.

4.3.3 Dirac Field in Coulomb Potential

After the substitution (4.70) into (4.69), we find the Dirac equation in the Coulomb potential (4.66):

$$\left[\left(E + \frac{Z\alpha}{r} \right) \gamma^0 + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} - M \right] \psi_E(\mathbf{x}) = 0. \tag{4.94}$$

In order to find the energy spectrum it is useful to establish contact with the Klein-Gordon case. Multiplying (4.94) by the operator

$$\left(E+\frac{Z\alpha}{r}\right)\gamma^0+i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+M, \tag{4.95}$$

we obtain

$$\left[\left(E+\frac{Z\alpha}{r}\right)^2+\boldsymbol{\nabla}^2-i\gamma^0\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}\frac{Z\alpha}{r}-M^2\right]\psi_E(\mathbf{x})=0., \tag{4.96}$$

In the chiral representation, 4×4 -matrix $\gamma^0\boldsymbol{\gamma}=\boldsymbol{\alpha}$ has a diagonal block form (3.514). We therefore decompose

$$\psi_E(\mathbf{x})=\left(\begin{array}{c}\xi_E(\mathbf{x})\\ \eta_E(\mathbf{x})\end{array}\right), \tag{4.97}$$

and find the equation for the upper two-component spinors

$$\left[\left(E+\frac{Z\alpha}{r}\right)^2+\boldsymbol{\nabla}^2+i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\frac{Z\alpha}{r}-M^2\right]\xi_E(\mathbf{x})=0, \tag{4.98}$$

and the same equation for $\eta_E(\mathbf{x})$ with i replaced by $-i$. Expressing $\boldsymbol{\nabla}^2$ via (4.72) and writing $\boldsymbol{\nabla}\,1/r=-\hat{\mathbf{x}}/r^2$, we obtain the differential equation

$$\left[-\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\hat{\mathbf{L}}^2-Z^2\alpha^2+iZ\alpha\boldsymbol{\sigma}\hat{\mathbf{x}}}{r^2}-\frac{2Z\alpha E}{r}-(E^2-M^2)\right]\xi_E(\mathbf{x})=0, \tag{4.99}$$

and a corresponding equation for $\eta_E(\mathbf{x})$.

Due to the rotation invariant of $\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}$, the total angular momentum

$$\hat{\mathbf{J}}=\hat{\mathbf{L}}+\mathbf{S}=\hat{\mathbf{L}}+\frac{\boldsymbol{\sigma}}{2} \tag{4.100}$$

commutes with the differential operator in (4.99). Thus we can diagonalize $\hat{\mathbf{J}}^2$ and $\hat{J}_3$ with eigenvalues $j(j+1)$ and m. For a fixed value of $j=\frac{1}{2},1,\frac{3}{2},\dots$, the orbital angular momentum can have the value $l_+=j+\frac{1}{2}$ and $l_-=j-1/2$. The two states have opposite parities. The operator $\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}$ is a pseudoscalar and must necessarily change the parities. Since the square of $\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}$ is the unit matrix, its eigenvalues must be ±1. Moreover, the unit vector x changes necessarily the parity and thus l. Thus, in the two-component Hilbert space of fixed quantum numbers j and m with orbital angular momenta $l=l_\pm=j\pm1/2$, the diagonal matrix elements vanish

$$\langle jm,+|\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}|jm,+\rangle=0,\qquad\langle jm,-|\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}|jm,-\rangle=0. \tag{4.101}$$

For the off-diagonal elements we easily calculate

$$\langle jm,+|\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}|jm,-\rangle=1,\qquad\langle jm,-|\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}|jm,+\rangle=-1. \tag{4.102}$$

The central parentheses in (4.99) have therefore the matrix elements

$$\left(\mathbf{L}^2 - Z^2\alpha^2 \pm iZ\alpha\hat{\mathbf{x}}\right) = \begin{pmatrix} (j+\frac{1}{2})(j+\frac{3}{2}) - Z^2\alpha^2 & \pm iZ\alpha \\ \pm iZ\alpha & (j-\frac{1}{2})(j+\frac{1}{2}) - Z^2\alpha^2 \end{pmatrix}. \tag{4.103}$$

In analogy with the Klein-Gordon case, we denote the eigenvalues of this matrix by $\lambda(\lambda+1)$. The corresponding values of λ are found to be

$$\lambda_+ = \left[\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2\right]^{1/2}, \quad \lambda_- = \lambda_+ - 1. \tag{4.104}$$

These may be written as

$$\lambda_\pm = j \pm \frac{1}{2} - \delta_j \tag{4.105}$$

with

$$\delta_j = j + \frac{1}{2} - \left[\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2\right]^{1/2} = \frac{Z^2\alpha^2}{2j+1} + \mathcal{O}(Z^4\alpha^4). \tag{4.106}$$

The radial quantum number n_r is again integer, and the combination of quantum numbers determining the energy is

$$n_r + \lambda_\pm + 1 = n_r + l_{\rm m} + 1 - \delta_l = n - \delta_j. \tag{4.107}$$

In terms of δ_j, the energies obey the same equation as in (4.93), so that we obtain

$$\begin{aligned} E_{nj} &= \frac{M}{\sqrt{1 + Z^2\alpha^2/(n-\delta_j)^2}} \\ &= M\left[1 - \frac{(Z\alpha)^2}{2n^2} + \frac{3}{8}\frac{(Z\alpha)^4}{n^4} - \frac{(Z\alpha)^4}{n^3(2j+1)} + \mathcal{O}(Z^6\alpha^6)\right]. \end{aligned} \tag{4.108}$$

The condition $n_r \geq 0$ implies that

$$\begin{array}{lcl} j \leq n - \frac{3}{2} & \multirow{2}{*}{for} & \lambda_+ = j + \frac{1}{2} - \delta_j, \\ j \leq n - \frac{1}{2} & & \lambda_- = j - \frac{1}{2} - \delta_j. \end{array} \tag{4.109}$$

For $n = 1, 2, 3, \ldots$, the total angular momentum runs through $j = \frac{1}{2}, \frac{3}{2}, \ldots, n - \frac{1}{2}$.

The spectrum of the hydrogen atom according to the Dirac theory is shown in Fig. 4.1. As a remnant of the O(4)-degeneracy of the levels with $l = 0, 1, 2, \ldots, n-1$ and fixed n in the Schrödinger spectrum, there is now a twofold degeneracy of levels of equal n and j, with adjacent l-values, which are levels of opposite parity. An exception is the highest total angular momentum $j = n - 1/2$ at each n which occurs only once. The lowest degenerate pair consists of the levels $2S_{1/2}$ and $2P_{1/2}$.[3]

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[3] Recall the notation in atomic physics for an electronic state: $n^{2S+1}L_J$, where n is the principal quantum number, L the orbital angular momentum, J the total angular momentum, and S the total spin. In a one-electron system such as the hydrogen atom, the trivial superscript $2S+1 = 2$ may be omitted.

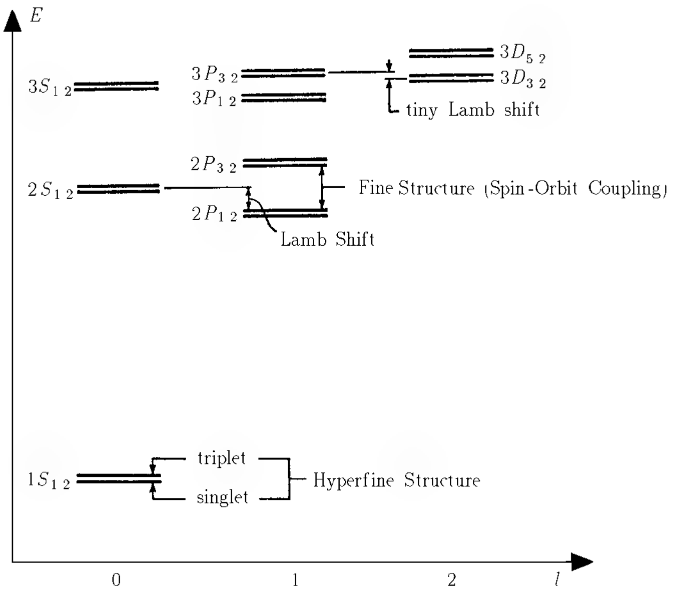

FIGURE 4.1 Hydrogen spectrum according to Dirac's theory. The splittings are shown only schematically. The fine-structure splitting of the $2P$-levels is about 10 times as big as the hyperfine splitting and Lamb shift.

It was an important experimental discovery to find that this prediction is wrong. There is a splitting of about 10% of the fine-structure splitting. This is called the *Lamb shift*. Its explanation is one of the early triumphs of quantum electrodynamics, which will be discussed in detail in Chapter .

As in the Klein-Gordon case, there are complex energies, here for $Z > 137$, with $S_{1/2}$ being the first level to become complex.

An important correct prediction of the Dirac theory is the presence of fine structure. States with the same n and l but with different j are split apart by the forth term in Eq. (4.108) $-MZ^4\alpha^4n^3/(2j+1)$. For the states $2P_{1/2}$ and $2P_{3/2}$, the splitting is

$$\Delta_{\rm fine}E_{2P} = \frac{Z^4\alpha^2}{32}\alpha^2 M. \tag{4.110}$$

In a hydrogen atom, this is equal to

$$\Delta_{\rm fine}E_{2P} = 3.10.95 \text{ GHz}. \tag{4.111}$$

Thus it is roughly of the order of the splitting caused by the interaction of the magnetic moment of the electron with that of the proton, the so-called *hyperfine-splitting*. This is for $2S^{1/2}, 2P^{1/2}$, and $2P^{3/2}$ levels approximately equal to 1, 1/8, 1/24, 1/60 times 1 420 MHz.[4]

In a hydrogen atom, the electronic motion is only slightly relativistic, the velocities being of the order αc, i.e., only about 1% of the light velocity. If one is not only interested in the spectrum but also in the wave functions it is advantageous to solve directly the Dirac equation (4.94) with the gamma matrices in the Dirac representation (3.501). Multiplying (4.94) by γ^0 and inserting for $\gamma^0\boldsymbol{\gamma} = \boldsymbol{\alpha}$ the Dirac matrix (3.513), we obtain

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[4] See H.A. Bethe and E.E. Salpeter in *Encyclopedia of Physics (Handbuch der Physik) 335*, Springer, Berlin, 1957, p. 196.

$$\begin{pmatrix} E - M + \dfrac{Z\alpha}{r} & i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} \\ i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} & E + M + \dfrac{Z\alpha}{r} \end{pmatrix} \begin{pmatrix} \xi_E(\mathbf{x}) \\ \eta_E(\mathbf{x}) \end{pmatrix} = 0. \tag{4.112}$$

This is of course just the time-independent version of (3.520) extended by the Coulomb potential according to the minimal substitution rule (4.70). To lowest order in α, the lower spinor is related to the upper by

$$\eta_E(\mathbf{x}) \approx -i\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}}{2M}\xi_E(\mathbf{x}). \tag{4.113}$$

We may take care of rotational symmetry of the system by splitting the spinor wave functions into radial and angular parts

$$\psi_E(\mathbf{x}) = \begin{pmatrix} i\dfrac{G_{jl}(r)}{r}\; y^l_{j,m}(\theta,\phi) \\ \dfrac{F_{jl}(r)}{r}\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}\; y^l_{j,m}(\theta,\phi) \end{pmatrix}, \tag{4.114}$$

where $y^l_{j,m}(\theta,\phi)$ denotes the *spinor spherical harmonics*. They are composed from the ordinary spherical harmonics $Y_{lm}(\theta,\varphi)$ and the basis spinors $\chi(s_3)$ of (3.401) via *Clebsch-Gordan coefficients* (see Appendix 3C):

$$y^l_{j,m}(\theta,\phi) = \langle j,m|l,m';\tfrac{1}{2},s_3\rangle Y_{lm'}(\theta,\varphi)\chi(s_3). \tag{4.115}$$

The derivation is given in Appendix 4A.

The explicit form of the spinor spherical harmonics (4.115) is for $l = l_\pm$:

$$y^{l_+}_{j,m}(\theta,\varphi) = \frac{1}{\sqrt{2l_+ + 1}} \begin{pmatrix} \sqrt{l_+ - m + \frac{1}{2}}Y_{l_+,m-\frac{1}{2}}(\theta,\varphi) \\ -\sqrt{l_+ + m + \frac{1}{2}}Y_{l_+,m+\frac{1}{2}}(\theta,\varphi) \end{pmatrix}, \tag{4.116}$$

$$y^{l_-}_{j,m}(\theta,\varphi) = \frac{1}{\sqrt{2l_- + 1}} \begin{pmatrix} \sqrt{l_- + m + \frac{1}{2}}Y_{l_-,m-\frac{1}{2}}(\theta,\varphi) \\ \sqrt{l_- - m + \frac{1}{2}}Y_{l_-,m+\frac{1}{2}}(\theta,\varphi) \end{pmatrix}. \tag{4.117}$$

The differential equations for the radial functions $F_{jl}(r)$ and $G_{jl}(r)$ are

$$\left(E - M + \frac{Z\alpha}{r}\right)G_{jl}(r) = -\frac{d}{dr}F_{jl}(r) \mp (j+1/2)\frac{1}{r}F_{jl}(r), \tag{4.118}$$

$$\left(E + M + \frac{Z\alpha}{r}\right)F_{jl}(r) = \frac{d}{dr}G_{jl}(r) \mp (j+1/2)\frac{1}{r}G_{jl}(r). \tag{4.119}$$

To solve these, dimensionless variables $\rho \equiv 2r/\lambda$ are introduced, with $\lambda = 1/\sqrt{M^2-E^2}$, writing

$$F(r) = \sqrt{1-E/M}e^{-\rho/2}(F_1-F_2)(\rho),\; G(r) = \sqrt{1+E/M}e^{-\rho/2}(F_1+F_2)(\rho). \tag{4.120}$$

The functions $F_{1,2}(\rho)$ satisfy a degenerate hypergeometric differential equation of the form

$$\left[\rho\frac{d^2}{d\rho^2}+(b-\rho)\frac{d}{d\rho}-a\right]F(a,b;\rho)=0, \tag{4.121}$$

and the solutions are

$$\begin{aligned} F_2(\rho) &= \rho^l F(\gamma - Z\alpha E\lambda, 2\gamma+1;\rho), \\ F_1(\rho) &= \rho^l \frac{\gamma - Z\alpha E\lambda}{-1/\lambda + Z\alpha E\lambda} F(\gamma+1-Z\alpha E\lambda, 2\gamma+1;\rho). \end{aligned} \tag{4.122}$$

The constant γ is Einstein's gamma parameter $\gamma = \sqrt{1-v^2/c^2}$ for the atomic unit velocity $v = Z\alpha c$. It has the expansion $\gamma = 1 - Z^2\alpha^2/2$,

As an example, we write down explicitly the ground state wave functions of the $1S^{1/2}$ state:

$$\psi_{1S^{1/2},\pm\frac{1}{2}} = \sqrt{\frac{(2MZ\alpha)^3}{4\pi}\frac{1+\gamma}{2\Gamma(1+2\gamma)}\frac{e^{-mZ\alpha r}}{(2MZ\alpha)^{1-\gamma}}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ i\frac{1-\gamma}{Z\alpha}\cos\theta & i\frac{1-\gamma}{Z\alpha}\sin\theta e^{-i\varphi} \\ i\frac{1-\gamma}{Z\alpha}\sin\theta e^{i\varphi} & -i\frac{1-\gamma}{Z\alpha}\cos\theta \end{pmatrix}. \tag{4.123}$$

The first column is for $m = 1/2$, the second for $m = -1/2$. For small α, Einstein's gamma parameter has the expansion $\gamma = 1 - Z^2\alpha^2/2$, and we see that in the $\alpha \to 0$, the upper components of the spinor wave functions tend to the nonrelativistic Schrödinger wave function $2\sqrt{(Z\alpha M)^3/4\pi}e^{-\rho}$ multiplied by Pauli spinors (3.401). In general,

$$\xi^l_{j,m}(\mathbf{x}) = \langle j,m|l,m;\tfrac{1}{2},s_3\rangle\psi_{nlm}(\mathbf{x})\chi(s_3). \tag{4.124}$$

The lower, small components vanish.

Appendix 4A Spinor Spherical Harmonics

Equation (4.115) defines spinor spherical harmonics. In these, an orbital wave function of angular momentum $l_\pm$ is coupled with spin 1/2 to a total angular momentum $j = l_\mp \pm 1/2$. For the configurations $j = l_- + 1/2$ with $m_2 = -1/2$ the recursion relation (3C.20) for the Clebsch-Gordan coefficients $\langle s_1 m_1; s_2 m_2|sm\rangle$, simplifies by having no second term. Inserting $s_1 = l_-$, $s_2 = 1/2$ and $s = j = l_- + 1/2$, we find

$$\langle l_-, m+\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}|l_-+\tfrac{1}{2}, m\rangle = \sqrt{\frac{l_- - m + 1/2}{l_- - m + 3/2}}\langle l_-, m-\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}|l_-+\tfrac{1}{2}, m-1\rangle. \tag{4A.1}$$

This has to be iterated with the initial condition

$$\langle l_-, -l_-; \tfrac{1}{2}, -\tfrac{1}{2} | l_- + \tfrac{1}{2}, -l_- - \tfrac{1}{2} \rangle = 1, \tag{4A.2}$$

which follows from the fact that the state $\langle l_-, -l_-; \frac{1}{2}, -\frac{1}{2}\rangle$ carries a unique magnetic quantum number $m = -l_- - 1/2$ of the irreducible representation of total angular momentum $s = j = l_- + 1/2$. The result of the iteration is

$$\langle l_+, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_+ - \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_+ - m + 1/2}{2l_+ + 1}}. \tag{4A.3}$$

Similarly we may simplify the recursion relation (3C.21) for the configurations $j = l_+ - 1/2$ with $m_2 = 1/2$ to

$$\langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_- + m + 1/2}{l_- + m + 3/2}} \langle l_-, m + \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m + 1 \rangle, \tag{4A.4}$$

and iterating this with the initial condition

$$\langle l_-, \, l_-; \tfrac{1}{2} n \tfrac{1}{2} | l_- + \tfrac{1}{2}, \, l_- + \tfrac{1}{2} \rangle = 1, \tag{4A.5}$$

which expresses the fact that the state $\langle l_- \, l_-; \frac{1}{2} \frac{1}{2}\rangle$ is the state of maximal magnetic quantum number $m = l_- + 1/2$ of the irreducible representation of total angular momentum $s = j = l_- + 1/2$. The result of the iteration is

$$\langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_+ + \tfrac{1}{2}, m \rangle = \sqrt{\frac{l_+ + m + 1/2}{2l_- + 1}}. \tag{4A.6}$$

Inserting (4A.3) and (4A.6) the expression (4.115) for the spinor spherical harmonic of total angular momentum $j = l_- + 1/2$, which now reads

$$\begin{aligned} y^{l_-}_{j,m}(\theta, \phi) &= \langle l_-, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle \quad Y_{l\,m-1/2}(\theta, \phi) \chi(\tfrac{1}{2}) \\ &+ \langle l_- \, m + \tfrac{1}{2}; \tfrac{1}{2} \; - \tfrac{1}{2} | l_- + \tfrac{1}{2}, m \rangle \; Y_{l\,m+1/2}(\theta, \phi) \chi(-\tfrac{1}{2}), \end{aligned} \tag{4A.7}$$

and separating the spin-up and spin-down components, we obtain precisely (4.117).

In order to find corresponding result for $j = l_+ - 1/2$, we use the orthogonality relation for states with the same l but different $j = l \pm 1/2$:

$$\langle l + \tfrac{1}{2}, m | l - \tfrac{1}{2}, m \rangle = 0. \tag{4A.8}$$

Inserting a complete set of states in the direct product space yields

$$\begin{aligned} &\langle l + \tfrac{1}{2}, m | l, m - \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2} \rangle \langle l m - \tfrac{1}{2}; \tfrac{1}{2} \tfrac{1}{2} | l - \tfrac{1}{2}, m \rangle \\ &+ \langle l + \tfrac{1}{2}, m | l, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} \rangle \langle l, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} | l - \tfrac{1}{2}, m \rangle = 0. \end{aligned} \tag{4A.9}$$

Together with (4A.3) and (4A.6) we find

$$\begin{aligned}
\langle l_+ .m-\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2}|l_+ {-}\tfrac{1}{2},m\rangle &= \sqrt{\frac{l_+ + m + 1/2}{2l_+ + 1}}, \\
\langle l_+ ,m+\tfrac{1}{2};\tfrac{1}{2},-\tfrac{1}{2}|l_+ {-}\tfrac{1}{2},m\rangle &= -\sqrt{\frac{l_+ - m + 1/2}{2l_+ + 1}},
\end{aligned} \tag{4A.10}$$

With this, the expression (4.115) for the spinor spherical harmonics written as

$$\begin{aligned}
y^{l_+}_{j,m}(\theta,\phi) &= \langle l_+ ,m-\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2}|l_+ {-}\tfrac{1}{2},m\rangle \;\; Y_{l,m-1/2}(\theta,\phi)\chi(\tfrac{1}{2}) \\
&+ \langle l_+ ,m+\tfrac{1}{2};\tfrac{1}{2},-\tfrac{1}{2}|l_+ {-}\tfrac{1}{2},m\rangle \, Y_{l,m+1/2}(\theta,\phi)\chi(-\tfrac{1}{2})
\end{aligned} \tag{4A.11}$$

has the components given in (4.116).

5

Quantization of Relativistic Free Fields

Following the field quantization rules developed Chapter 2 from the N-body Schrödinger equation we now turn to quantizing free relativistic fields. The general rules were given in Sections 2.8 and 2.10 for bosons and fermions, respectively. Following these rules, we define for each field $\phi(\mathbf{x},t)$ in a classical Lagrangian $L(t)$ a canonical field momentum by the functional derivative (2.157) at a given time

$$\pi(\mathbf{x},t) = p_{\mathbf{x}}(t) = \frac{\delta L(t)}{\delta\dot{\phi}(\mathbf{x},t)}. \tag{5.1}$$

The fields are now made field operators by imposing the canonical equal-time commutation rules (2.141)

$$\begin{aligned} \left[\phi(\mathbf{x},t),\phi(\mathbf{x}',t)\right] &= 0, & (5.2)\\ \left[\pi(\mathbf{x},t),\pi(\mathbf{x}',t)\right] &= 0, & (5.3)\\ \left[\pi(\mathbf{x},t),\phi(\mathbf{x}',t)\right] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'). & (5.4) \end{aligned}$$

For fermions, there will be corresponding anticommutation rules.

In Eqs. (5.2)–(5.4) we have omitted the hat on top of the field operators, and we shall do so from here on everywhere, for brevity, since most field expressions will contain quantized fields. In the few cases where this is not the case and where it is not obvious that the fields are classical objects we shall explicitly state this. We shall also use natural units in which $c = 1$, $\hbar = 1$, except in some cases where cgs units are helpful.

Before implementing the commutation rules explicitly it is useful to note that all free Lagrangians constructed in the last chapter are local in the sense that they are given by volume integrals over a Lagrangian density

$$L(t) = \int d^3x\, \mathcal{L}(\mathbf{x},t), \tag{5.5}$$

where $\mathcal{L}(\mathbf{x},t)$ is an ordinary function of the fields and their first spacetime derivatives. The functional derivative (5.1) may therefore be calculated as a partial derivative of the density $\mathcal{L}(x) = \mathcal{L}(\mathbf{x},t)$:

$$\pi(x) = \frac{\partial\mathcal{L}(x)}{\partial\dot{\phi}(x)}, \tag{5.6}$$

Similarly, the Euler-Lagrange equations may be written down using only partial derivatives

$$\partial^\mu \frac{\partial \mathcal{L}(x)}{\partial[\partial^\mu \phi(x)]} = \frac{\partial \mathcal{L}(x)}{\partial \phi(x)}. \tag{5.7}$$

Here and in the sequel we employ a four-vector notation for all spacetime objects such as $x = (x^0, \mathbf{x})$ where $x^0 = ct$ coincides with the time t in natural units.

The locality is an important property of all present-day quantum field theories of elementary particles. The spacetime derivatives appear usually only in quadratic terms. Since a derivative measures the difference of the field between neighboring spacetime points, the field described by a local Lagrangian propagates through spacetime via a "nearest-neighbor coupling". In field-theoretic models of solid-state systems, such couplings are useful lowest approximations to more complicated short-range interactions. In field theories of elementary particles, the locality is an essential ingredient which seems to be present in all fundamental theories.

5.1 SCALAR FIELDS

We begin by quantizing a scalar field satisfying the Klein-Gordon equation (3.163):

$$(-\partial^2 - M^2)\phi(x) = 0. \tag{5.8}$$

5.1.1 Real Case

The Lagrangian density of the field was given in Eq. (3.160). As we shall understand in Subsec. 5.1.6 (and understand more deeply in Subsec. 6.11.1), the real field describes *neutral scalar particles*. For the canonical quantization we must use the Lagrangian density (3.161) in which only first derivatives of the field occur:

$$\mathcal{L}(x) = \frac{1}{2}\left[\partial\phi(x)\partial\phi(x) - M^2\phi^2(x)\right]. \tag{5.9}$$

5.1.2 Field Quantization

According to the rule (5.6), the canonical momentum of the field is

$$\pi(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{\phi}(x)} = \partial^0\phi(x) = \dot{\phi}(x). \tag{5.10}$$

As in the case of non-relativistic fields, the quantization rules (5.2)–(5.4) will eventually render a multiparticle Hilbert space. To find it we expand the field operator $\phi(x, t)$ in normalized plane-wave solutions (3.172) of the field equation (5.8):

$$\phi(x) = \sum_{\mathbf{p}} \left[f_{\mathbf{p}}(x)a_{\mathbf{p}} + f^*_{\mathbf{p}}(x)a^\dagger_{\mathbf{p}}\right]. \tag{5.11}$$

Observe that in contrast to a corresponding expansion (2.210) of the nonrelativistic Schrödinger field, the right-hand side contains operators for the creation and annihilation of particles. This is an automatic consequence of the fact that the quantization of a real field must lead to a hermitian field operator. This has the physical consequence, that a quantized real field theory which can only exists in the relativistic setting, will necessarily allow for the creation and annihilation of particles,

Inserting the explicit wave functions (3.172), the expansion reads

$$\phi(x)=\sum_{\mathbf{p}}\frac{1}{\sqrt{2p^0V}}(e^{-ipx}a_{\mathbf{p}}+e^{ipx}a^\dagger_{\mathbf{p}}), \tag{5.12}$$

Since the zeroth component of the four-momentum p^μ in the exponent is on mass shell, we should write px more explicitly as $px=\omega_{\mathbf{p}}t-\mathbf{px}$. However, the notation px is shorter, and there is little danger of confusion. If this is the case, we shall state the on- or off-shell property of p^0 explicitly.

The expansions (5.11) and (5.12) are complete. The first may be solved for $a_{\mathbf{p}}$ and $a^\dagger_{\mathbf{p}}$ with the help of the orthonormality relations (3.170) to obtain we obtain directly

$$a^\dagger_{\mathbf{p}}=(\phi_{\mathbf{p}}(t),\phi(t)),\qquad a_{\mathbf{p}}=-(\phi^*_{\mathbf{p}}(t),\phi(t)). \tag{5.13}$$

More explicitly, this can be written as

$$\left\{\begin{array}{c}a_{\mathbf{p}}\\ a^\dagger_{\mathbf{p}}\end{array}\right\}=e^{\pm ip^0x_0}\frac{1}{\sqrt{2Vp^0}}\int d^3x\,e^{\mp i\mathbf{px}}\left[\pm i\pi(x)+p^0\phi(x)\right]. \tag{5.14}$$

where we have inserted $\pi(x)=\dot\phi(x)$.

Using the canonical field commutation rules (5.2)–(5.4) between $\phi(x)$ and $\pi(x)$, we find for the coefficients of the plane-wave expansion (5.12) the commutation relations

$$\begin{aligned}\left[a_{\mathbf{p}},a_{\mathbf{p}'}\right] &= \left[a^\dagger_{\mathbf{p}},a^\dagger_{\mathbf{p}'}\right]=0,\\ \left[a_{\mathbf{p}},a^\dagger_{\mathbf{p}'}\right] &= \delta_{\mathbf{p},\mathbf{p}'},\end{aligned} \tag{5.15}$$

making them creation and annihilation operators of particles of momentum $\mathbf{p}$ on a vacuum state $|0\rangle$ defined by $a_{\mathbf{p}}|0\rangle=0$. Conversely, reinserting (5.15) into (5.12) we verify the original local field commutation rules (5.2)–(5.4).

If the spatial volume V is infinite, we may use in (5.11) the wave functions (3.173) with continuous momenta, and work with a Fourier integral for the plane-wave decomposition

$$\phi(x)=\int\frac{d^3p}{(2\pi)^3}\frac{1}{2p^0}\left[e^{-ipx}\mathrm{a}_{\mathbf{p}}+e^{ipx}\mathrm{a}^\dagger_{\mathbf{p}}\right], \tag{5.16}$$

with the identification [recall (2.218)]

$$\mathrm{a}_{\mathbf{p}}=\sqrt{2p^0V}a_{\mathbf{p}},\qquad \mathrm{a}^\dagger_{\mathbf{p}}=\sqrt{2p^0V}a^\dagger_{\mathbf{p}}. \tag{5.17}$$

The expansion is now inverted to

$$\left\{ \begin{array}{c} \mathrm{a}_{\mathbf{p}} \\ \mathrm{a}^{\dagger}_{\mathbf{p}} \end{array} \right\} = e^{\pm i p^0 x_0} \int d^3x\, e^{\mp i \mathbf{p}\mathbf{x}} \left[\pm i\pi(x) + p^0 \phi(x) \right]. \tag{5.18}$$

This can of course be written in the same form as in (5.13) using the orthogonality relations (3.174) for continuous-momentum wave functions (3.173):

$$\mathrm{a}^{\dagger}_{\mathbf{p}} = (\mathrm{f}_{\mathbf{p}}, \phi)_t, \qquad \mathrm{a}_{\mathbf{p}} = -(\mathrm{f}^{*}_{\mathbf{p}}, \phi)_t. \tag{5.19}$$

In the expansion (5.11), the commutators (5.15) hold with the replacement [recalling the definition (1.122), and keeping $\hbar$, to be explicit]

$$\delta_{\mathbf{p},\mathbf{p}'} \rightarrow 2p^0\, \delta^{(3)}(\mathbf{p}-\mathbf{p}') = 2p^0 (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p}-\mathbf{p}'), \tag{5.20}$$

In the following we shall always use sums over $\mathbf{p}$. In all formulas, we can always go over to the continuum limit by replacing the sums as in (2.259) by phase space integrals :

$$\begin{aligned} \sum_{\mathbf{p}} \quad &\rightarrow \quad \int d^3p \frac{V}{(2\pi\hbar)^3}, \\ \delta_{\mathbf{p},\mathbf{p}'} \quad &\rightarrow \quad \frac{(2\pi\hbar)^3}{V} \delta^{(3)}(\mathbf{p}-\mathbf{p}'). \end{aligned} \tag{5.21}$$

After the replacement (5.17), the volume V disappears in most relevant quantities expressed in terms of creation and annihilation $a(\mathbf{p})$ and $a^{\dagger}(\mathbf{p})$.

A single-particle state of a fixed momentum $\mathbf{p}$ is created by

$$|\mathbf{p}\rangle = a^{\dagger}_{\mathbf{p}}|0\rangle. \tag{5.22}$$

Its wave function is obtained from the matrix elements of the field

$$\begin{aligned} \langle 0|\phi(x)|\mathbf{p}\rangle &= \frac{1}{\sqrt{2Vp^0}} e^{-ipx} = f_{\mathbf{p}}(x), \\ \langle \mathbf{p}|\phi(x)|0\rangle &= \frac{1}{\sqrt{2Vp^0}} e^{ipx} = f^{*}_{\mathbf{p}}(x). \end{aligned} \tag{5.23}$$

As in the nonrelativistic case, the second-quantized Hilbert space is obtained by applying the particle creation operators $a^{\dagger}_{\mathbf{p}}$ to the vacuum state $|0\rangle$, defined by $a^{\dagger}_{\mathbf{p}}|0\rangle = 0$, leading to states (2.220):

$$|n_{\mathbf{p}_1} n_{\mathbf{p}_2} \dots n_{\mathbf{p}_k}\rangle = \mathcal{N}^{S,A} (\hat{a}^{\dagger}_{\mathbf{p}_1})^{n_{\mathbf{p}_1}} \cdots (\hat{a}^{\dagger}_{\mathbf{p}_k})^{n_{\mathbf{p}_k}} |0\rangle, \tag{5.24}$$

Multiparticle wave functions are obtained by matrix elements of the type (2.222).

In an infinite volume, we shall sometimes use the single-particle states

$$|\mathbf{p}\rangle = \mathrm{a}^{\dagger}_{\mathbf{p}}|0\rangle. \tag{5.25}$$

with the vacuum $|0)$ defined by $a_{\mathbf{p}}|0) = 0$. These states satisfy the orthogonality relation

$$(\mathbf{p}'|\mathbf{p}) = 2p^0\,\delta^{(3)}(\mathbf{p}' - \mathbf{p}), \tag{5.26}$$

and have the wave functions

$$\begin{aligned}(0|\phi(x)|\mathbf{p}) &= e^{-ipx} = \mathrm{f}_{\mathbf{p}}(x),\\ (\mathbf{p}|\phi(x)|0) &= e^{ipx} \;= \mathrm{f}^*_{\mathbf{p}}(x).\end{aligned} \tag{5.27}$$

Energy of Free Neutral Scalar Particles

Due to the local structure (5.5) of the Lagrangian, also the Hamiltonian can be written as a volume integral

$$H = \int d^3x\,\mathcal{H}(x). \tag{5.28}$$

The Hamiltonian density is the Legendre transform of the Lagrangian density

$$\begin{aligned}\mathcal{H}(x) &= \pi(x)\partial^0\phi(x) - \mathcal{L}(x)\\ &= \frac{1}{2}[\partial^0\phi(x)]^2 + \frac{1}{2}[\partial_{\mathbf{x}}\phi(x)]^2 + \frac{M^2}{2}\phi^2(x).\end{aligned} \tag{5.29}$$

Inserting the expansion (5.12), we obtain the Hamilton operator

$$\begin{aligned}H &= \sum_{\mathbf{p},\mathbf{p}'}\left\{\frac{1}{2\sqrt{p^0p'^0}}\delta_{\mathbf{p},\mathbf{p}'}\left(p^0p'^0 + \mathbf{p}\cdot\mathbf{p}' + M^2\right)\left(a^\dagger_{\mathbf{p}}a_{\mathbf{p}'} + a_{\mathbf{p}}a^\dagger_{\mathbf{p}'}\right)\right.\\ &\quad\left.+\frac{1}{2\sqrt{p^0p'^0}}\delta_{\mathbf{p},-\mathbf{p}'}\left(-p^0p'^0 - \mathbf{p}\cdot\mathbf{p}' + M^2\right)\left[a^\dagger_{\mathbf{p}}a^\dagger_{\mathbf{p}'}e^{i(p^0+p'^0)t} + a_{\mathbf{p}}a_{\mathbf{p}'}e^{-i(p^0+p'^0)t}\right]\right\}\\ &= \sum_{\mathbf{p}} p^0\left(a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + \frac{1}{2}\right).\end{aligned} \tag{5.30}$$

The vacuum state $|0\rangle$ has an energy

$$E_0 \equiv \langle 0|H|0\rangle = \frac{1}{2}\sum_{\mathbf{p}} p^0 = \frac{1}{2}\sum_{\mathbf{p}}\omega_{\mathbf{p}}, \tag{5.31}$$

due to the zero-point oscillations of all the "oscillator quanta" in the second quantization formalism, the so-called *vacuum fluctuations* of the field. This energy is infinite. In most circumstances, however, this infinity is unobservable. It is therefore often subtraced out of the Hamiltonian, replacing H by

$$:H:\equiv H - \langle 0|H|0\rangle. \tag{5.32}$$

The double dots to the left-hand side define what is called the *normal product* form of H. It is obtained by the following prescription on the operators $a, a^\dagger$:
In an arbitrary product of creation and annihilation operators,

$$:a^\dagger\cdots a\cdots a^\dagger\cdots a:,$$

the double dots reorder this product in such a way that all creation operators stand to the left of all annihilation operators. For example,

$$:a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + a_{\mathbf{p}}a^\dagger_{\mathbf{p}}: = 2a^\dagger_{\mathbf{p}}a_{\mathbf{p}} \tag{5.33}$$

and

$$:H:= \sum_{\mathbf{p}} p^0 a^\dagger_{\mathbf{p}}a_{\mathbf{p}}. \tag{5.34}$$

In following this ad hoc procedure, care has to be taken that one is not dealing with phenomena which depend on the omitted zero-point oscillations. Gravitational interactions, for example, are sensitive to the zero-point energy. The infinity creates serious problems when trying to construct quantum field theories in the presence of a classical gravitational field, since the vacuum energy gives rise to an infinite cosmologcal constant, which experimentally seems to be zero. A possible solution of this problem will be appear later when quantizing the Dirac field in Section 5.3. We shall see in Eq. (5.235) that for the Dirac field, the vacuum energy has the same form as for the scalar field, but with an opposite sign. In fact, this sign change occurs for fields of any half-integer spin. In Section 5.8 we shall see that such spins are always associated with bosons and fermions, receptively. The sum of bosonic and fermionic vacuum energies is then

$$E^{\rm tot}_{\rm vac} = \frac{1}{2}\sum_{\mathbf{p},\rm bosons} p^0 - \frac{1}{2}\sum_{\mathbf{p},\rm fermions} p^0. \tag{5.35}$$

Expanding p^0 as

$$p^0 = \omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2} = |\mathbf{p}|\left(1 + \frac{1}{2}\frac{M^2}{\mathbf{p}^2} - \frac{1}{8}\frac{M^4}{\mathbf{p}^4} + \dots\right), \tag{5.36}$$

we see that the vacuum energy can be finite if the universe contains as many Bose fields as Fermi fields, and if the masses of the associated particles satisfy the sum rules

$$\begin{aligned}\sum_{\rm bosons} M^2 &= \sum_{\rm fermions} M^2,\\ \sum_{\rm bosons} M^4 &= \sum_{\rm fermions} M^4.\end{aligned} \tag{5.37}$$

The higher powers in M contribute with finite momentum sums in (5.35).

Even without the presence of fermions, there exist finite observable consequences of the vacuum energy, the famous *Casimir effect* and the *Van der Waals forces*) between different dielectric media, which will be discussed in Section 5.10.

5.1.3 Propagator of Free Scalar Particles

The free-particle propagator of the scalar field is obtained from the vacuum expectation

$$G(x,x') = \langle 0|T\phi(x)\phi(x')|0\rangle. \tag{5.38}$$

As for nonrelativistic fields, the propagator coincides with the Green function of the free-field equation. This follows from the explicit form of the time-ordered product

$$T\phi(x)\phi(x') \;=\; \Theta(x_0-x'_0)\phi(x)\phi(x')+\Theta(x'_0-x_0)\phi(x')\phi(x). \tag{5.39}$$

Multiplying $G(x,x')$ by the operator ∂^2, we obtain

$$\begin{aligned}\partial^2 T\phi(x)\phi(x') = T[\partial^2\phi(x)]\phi(x')& \\ +2\delta(x_0-x'_0)\left[\partial_0\phi(x),\phi(x')\right]+\delta'(x_0-x'_0)\left[\phi(x),\phi(x')\right].&\end{aligned} \tag{5.40}$$

The last term can be manipulated according to the usual rules of distributions: It is multiplied by an arbitrary smooth test function of x_0, say $f(x_0)$, and becomes after a partial integration:

$$\begin{aligned}&\int dx_0 f(x_0)\delta'(x_0-x'_0)[\phi(x),\phi(x')] = \\ &-\int dx_0 f'(x_0)\delta(x_0-x'_0)[\phi(x),\phi(x')]-\int dx_0 f(x_0)\delta(x_0-x'_0)[\dot\phi(x),\phi(x')].\end{aligned} \tag{5.41}$$

The first term on the right-hand side does not contribute since it contains the commutator of the fields only at equal-times, $[\phi(x),\phi(x')]_{x^0=x^{0\prime}}$, where it vanishes. Thus, dropping the test function $f(x_0)$, we have the equality between distributions

$$\delta'(x_0-x'_0)[\phi(x),\phi(x')] = -\delta(x_0-x'_0)[\dot\phi(x),\phi(x')], \tag{5.42}$$

and therefore with (5.4), (5.10), (5.38)–(5.40):

$$(-\partial^2-M^2)G(x,x') = i\delta(x_0-x'_0)\delta^{(3)}(\mathbf{x}-\mathbf{x}') = i\delta^{(4)}(x-x'). \tag{5.43}$$

To calculate $G(x,x')$ explicitly, we insert (5.12) and (5.39) into (5.38), and find

$$\begin{aligned}G(x,x') &= \Theta(x_0-x'_0)\frac{1}{2V}\sum_{\mathbf{p},\mathbf{p}'}\frac{1}{\sqrt{p^0p'^0}}e^{-i(px-p'x')}\langle 0|a_{\mathbf{p}}a^\dagger_{\mathbf{p}'}|0\rangle \\ &+ \Theta(x'_0-x_0)\frac{1}{2V}\sum_{\mathbf{p},\mathbf{p}'}\frac{1}{\sqrt{p^0p'^0}}e^{i(px-p'x')}\langle 0|a_{\mathbf{p}'}a^\dagger_{\mathbf{p}}|0\rangle \\ &= \Theta(x_0-x'_0)\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{-ip(x-x')}+\Theta(x'_0-x_0)\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{ip(x-x')}.\end{aligned} \tag{5.44}$$

It is useful to introduce the functions

$$G^{(\pm)}(x,x') = \sum_{\mathbf{p}}\frac{1}{2p^0V}e^{\mp ip(x-x')}, \tag{5.45}$$

They are equal to the commutators at arbitrary times of the positive- and negative-frequency parts of the field $\phi(x)$ which annihilate and create free single-particle states, respectively, defined by

$$\phi^{(+)}(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} e^{-ipx} a_{\mathbf{p}}, \qquad \phi^{(-)}(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0 V}} e^{ipx} a^\dagger_{\mathbf{p}}. \tag{5.46}$$

In terms of these,

$$G^{(+)}(x,x') = [\phi^{(+)}(x), \phi^{(-)}(x')], \qquad G^{(-)}(x,x') = -[\phi^{(-)}(x), \phi^{(+)}(x')] = G^{(-)}(x',x) \tag{5.47}$$

The commutators on the right-hand sides can of course also be replaced by the corresponding expectation values. As such, they may also be rewritten as follows:

$$G^{(\pm)}(x,x') = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} e^{\pm i\mathbf{p}(\mathbf{x}-\mathbf{x}')} G^{(\pm)}(\mathbf{p}, t-t'), \tag{5.48}$$

with

$$G^{(\pm)}(\mathbf{p}, t-t') \equiv e^{\mp ip^0(t-t')} \tag{5.49}$$

being expectation values

$$\begin{aligned} G^{(+)}(\mathbf{p}, t-t') &= \langle 0|a_{\mathbf{p}\,\mathrm{H}}(t) a^\dagger_{\mathbf{p}\,\mathrm{H}}(t')|0\rangle, \\ G^{(+)}(\mathbf{p}, t-t') &= \langle 0|a_{\mathbf{p}\,\mathrm{H}}(t') a^\dagger_{\mathbf{p}\,\mathrm{H}}(t)|0\rangle, \end{aligned} \tag{5.50}$$

of Heisenberg creation and annihilation operators [recall the definition (1.245), and (2.130)] of frequency $p^0 = \omega_{\mathbf{p}}$:

$$a_{\mathbf{p}\,\mathrm{H}}(t) \equiv e^{iHt} a_{\mathbf{p}} e^{-iHt} = e^{-ip^0 t} a_{\mathbf{p}}, \qquad a^\dagger_{\mathbf{p}\,\mathrm{H}}(t) \equiv e^{iHt} a^\dagger_{\mathbf{p}} e^{-iHt} = e^{ip^0 t} a^\dagger_{\mathbf{p}}. \tag{5.51}$$

In the infinite-volume limit, the functions (5.45) have the Fourier representation

$$G^{(\pm)}(x,x') = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} e^{\mp ip(x-x')}. \tag{5.52}$$

The full commutator $[\phi(x), \phi(x')]$ receives contributions from both functions and is given by

$$[\phi(x), \phi(x')] = G^{(+)}(x-x') - G^{(-)}(x-x') \equiv C(x-x'). \tag{5.53}$$

The right-hand side defines the *commutator function*, which has the Fourier representation

$$C(x-x') = -i \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \sin[p^0(x^0 - x'^0)]. \tag{5.54}$$

This representation is convenient for verifying the canonical equal-time commutation rules (5.2) and (5.4) which imply that

$$C(x-x') = 0, \qquad \dot{C}(x-x') = -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \quad \text{for } x^0 = x'^0. \tag{5.55}$$

Indeed, for $x^0 = x'^0$, the integrand is zero, so that the integral vanishes. The time derivative of $C(x - x')$ removes p^0 in the denominator, leading at $x^0 = x'^0$ directly to the Fourier representation of the spatial δ-function.

Another way of writing (5.54) is via a formal off-shell momentum integral

$$C(x, x') = \int \frac{d^4p}{(2\pi)^4} 2\pi\Theta(p^0)\delta(p^2 - M^2)e^{-ip(x-x')} \tag{5.56}$$

In contrast to the Feynman propagator which satisfies the inhomogenous Klein-Gordon equation, the commutator function (5.53) satisfies the homogenous equation:

$$(-\partial^2 - M^2)C(x - x') = 0. \tag{5.57}$$

The Fourier representation (5.56) has obviously this property, since multiplication from the left by the Klein-Gordon operator produces an integrand proportional to $(p^2 - M^2)\delta(p^2 - M^2) = 0$.

The equality of the two expressions (5.54) and (5.56) follows from the property of the δ-function

$$\delta(p^2 - M^2) = \delta(p^{02} - \omega_{\mathbf{p}}^2) = \frac{1}{2\omega_{\mathbf{p}}}[\delta(p^0 - \omega_{\mathbf{p}}) + \delta(p^0 + \omega_{\mathbf{p}})]. \tag{5.58}$$

which selectsfrom the integral over p^0 containing $\Theta(p^0)$ precisely the on-shell value $p^0 = \omega_{\mathbf{p}}$ in agreement with (5.54).

In terms of the functions $G^{(\pm)}(x, x')$, the propagator can be written as

$$G(x, x') = G(x, x') = \Theta(x_0 - x'_0)G^{(+)}(x, x') + \Theta(x'_0 - x_0)G^{(-)}(x, x'). \tag{5.59}$$

As follows from (5.52) and (5.59), all three functions $G(x, x')$, $G^{(+)}(x, x')$, and $G^{(-)}(x, x')$ depend only on $x - x'$, thus exhibiting the translational invariance of the vacuum state. In the following, we shall therefore always write one argument $x - x'$ instead of x, x'.

As in the nonrelativistic case, it is convenient to use the integral representation (1.222) for the Θ-functions

$$\begin{aligned} \Theta(x_0 - x'_0) &= \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{i}{E - p^0 + i\eta} e^{-i(E-p^0)(x_0-x'_0)}, \\ \Theta(x'_0 - x_0) &= -\int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{i}{E + p^0 - i\eta} e^{-i(E+p^0)(x_0-x'_0)}, \end{aligned} \tag{5.60}$$

with an infinitesimal parameter $\eta > 0$, to reexpress $G(x, x')$ from (5.52), (5.49), and (5.59) more compactly as

$$G(x - x') = \int \frac{dE}{2\pi} \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} \left(\frac{i}{E - p^0 + i\eta} - \frac{i}{E + p^0 - i\eta} \right) e^{-iE(x_0-x'_0)+i\mathbf{p}(\mathbf{x}-\mathbf{x}')}, \tag{5.61}$$

where we have used the fact that p^0 is an even function of $\mathbf{p}$, thus permitting us to change the integration variables $\mathbf{p}$ to $-\mathbf{p}$ in the second integral. By combining the denominators we find

$$\int \frac{dE}{2\pi} \frac{d^3p}{(2\pi)^3} \frac{i}{E^2 - \mathbf{p}^2 - M^2 + i\eta} e^{-iE(x_0-x_0')+i\mathbf{p}(\mathbf{x}-\mathbf{x}')}. \tag{5.62}$$

This has a relativistic invariant form in which it is useful to rename E as p^0, and write

$$G(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')}. \tag{5.63}$$

Note that in this expression, p^0 is integrated over the entire p^0-axis. In contrast to all earlier formulas in this section, it is no longer constraint to satisfy the mass shell conditions $(p^0)^2 = p^{0^2} = \mathbf{p}^2 + M^2$.

The integral representation (5.63) shows very directly that $G(x, x')$ is the Green function of the free-field equation (5.8). An application of the differential operator $(-\partial^2 - M^2)$ cancels the denominator in the integrand and yields

$$\begin{aligned} (-\partial^2 - M^2) G(x-x') &= \int \frac{d^4p}{(2\pi)^4} (p^2 - M^2) \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')} \\ &= i\delta^{(4)}(x-x'). \end{aligned} \tag{5.64}$$

This calculation gives rise to a simple *mnemonic rule* for finding the Green function: for an arbitrary free-field theory: We write the Lagrangian density (5.9) as

$$\mathcal{L}(x) = \frac{1}{2}\phi(x) L(i\partial)\phi(x), \tag{5.65}$$

with the differential operator

$$L(i\partial) \equiv (-\partial^2 - M^2). \tag{5.66}$$

The Euler-Lagrange equation (5.8) can then be written simply as

$$L(i\partial)\phi(x) = 0. \tag{5.67}$$

The Green function is now the Fourier transform of the inverse of $L(i\partial)$

$$G(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{L(p)} e^{-ip(x-x')}, \tag{5.68}$$

with an infinitesimal $-i\eta$ added to the mass of the particle. This rule can directly be generalized to all other free-field theories to be discussed in the sequel.

5.1.4 Complex Case

Here we use the Lagrangian (3.162):

$$\mathcal{L}(x) = \partial^\mu \phi^*(x) \partial_\mu \phi(x) - M^2 \phi^*(x)\phi(x), \tag{5.69}$$

As we shall later see in Subsec. 5.1.6 (and understand more deeply in Subsec. 6.11.1), the complex field describes *charged scalar particles*.

Field Quantization

According to the canonical rules, the complex field possess complex canonical momenta

$$\begin{aligned}\pi_\phi(x) &\equiv \pi(x) \equiv \frac{\partial\mathcal{L}(x)}{\partial[\partial^0\phi(x)]} = \partial^0\phi^*(x),\\ \pi_{\phi^*}(x) &\equiv \pi^*(x) \equiv \frac{\partial\mathcal{L}(x)}{\partial[\partial^0\phi^*(x)]} = \partial^0\phi(x).\end{aligned} \tag{5.70}$$

The associated operators are required to satisfy the equal-time commutation rules

$$\begin{aligned}[\pi(\mathbf{x},t),\phi(\mathbf{x}',t)] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \qquad (5.71)\\ [\pi^\dagger(\mathbf{x},t),\phi^\dagger(\mathbf{x}',t)] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}').\end{aligned}$$

All other equal-time commutators vanish. We now expand the field operator into its Fourier components

$$\phi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}}\left(e^{-ipx}a_{\mathbf{p}} + e^{ipx}b^\dagger_{\mathbf{p}}\right), \tag{5.72}$$

where, in contrast to the real case (5.12), $b^\dagger_{\mathbf{p}}$ is no longer equal to $a^\dagger_{\mathbf{p}}$. The reader may wonder why we do not just use another set of annihilation operators $d_{-\mathbf{p}}$ rather than creation operators $b^\dagger_{\mathbf{p}}$. A negative sign in the momentum label would be appropriate since the associated wave function $f^*_{\mathbf{p}}(x) = e^{ipx}/\sqrt{2Vp^0}$ has a negative momentum. One formal reason for using $b^\dagger_{\mathbf{p}}$ instead of $d_{-\mathbf{p}}$ is that this makes the expansion (5.72) the straightforward generalization of the expansion (5.12) of the real field. A more physical reason will be seen below when discussing Eq. (5.81).

In analogy with (5.14), we invert (5.72) to find

$$\left\{\begin{array}{c} a_{\mathbf{p}} \\ b^\dagger_{\mathbf{p}} \end{array}\right\} = e^{\pm ip^0x_0}\sqrt{\frac{1}{2Vp^0}}\int d^3x\, e^{\mp i\mathbf{px}}\left[\pm i\pi^\dagger(x) + p^0\phi(x)\right], \tag{5.73}$$

and the corresponding hermitian-adjoint operators $a^\dagger_{\mathbf{p}}$ and $b_{\mathbf{p}}$.

From these equations we find the operators $a_{\mathbf{p}}$, $a^\dagger_{\mathbf{p}}$, $b_{\mathbf{p}}$, and $b^\dagger_{\mathbf{p}}$ all commute with each other, except for

$$\left[a_{\mathbf{p}}, a^\dagger_{\mathbf{p}'}\right] = \delta_{\mathbf{p},\mathbf{p}'}, \qquad \left[b_{\mathbf{p}}, b^\dagger_{\mathbf{p}'}\right] = \delta_{\mathbf{p},\mathbf{p}'}. \tag{5.74}$$

There are two types of particle states, created by

$$\begin{aligned}|\mathbf{p}\rangle \equiv a^\dagger_{\mathbf{p}}|0\rangle, &\quad |\bar{\mathbf{p}}\rangle \equiv b^\dagger_{\mathbf{p}}|0\rangle,\\ \langle\mathbf{p}| \equiv \langle 0|a_{\mathbf{p}}, &\quad \langle\bar{\mathbf{p}}| \equiv \langle 0|b_{\mathbf{p}}.\end{aligned} \tag{5.75}$$

They have the wave functions

$$\begin{aligned}\langle 0|\phi(x)|\mathbf{p}\rangle &= \frac{1}{\sqrt{2Vp^0}}e^{-ipx} = f_{\mathbf{p}}(x), & \langle 0|\phi^\dagger(x)|\bar{\mathbf{p}}\rangle &= \frac{1}{\sqrt{2Vp^0}}e^{-ipx} = f_{\mathbf{p}}(x),\\ \langle\bar{\mathbf{p}}|\phi(x)|0\rangle &= \frac{1}{\sqrt{2Vp^0}}e^{ipx} = f^*_{\mathbf{p}}(x), & \langle\mathbf{p}|\phi^\dagger(x)|0\rangle &= \frac{1}{\sqrt{2Vp^0}}e^{ipx} = f^*_{\mathbf{p}}(x).\end{aligned} \tag{5.76}$$

We are now ready to justify why we associated with the second term in the expansion (5.72) a creation operator $b^\dagger_{\mathbf{p}}$ rather than an annihilation operator $d_{-\mathbf{p}}$. First, this is in closer analogy with the real field in (5.12) which contains a creation operator $a^\dagger_{\mathbf{p}}$ accompanied by the negative-frequency wave function e^{ipx}. Second, only the above choice leads to commutation rules (5.74) for $b_{\mathbf{p}}, b^\dagger_{\mathbf{p}}$ with the correct sign. The choice $d_{\mathbf{p}}$ would have led to the commutator $[d_{\mathbf{p}}, d^\dagger_{\mathbf{p}'}] = -\delta_{\mathbf{p},\mathbf{p}'}$. For the second-quantized Hilbert space, this would imply the norm of the states created by $d^\dagger_{\mathbf{p}}$ to be negative. Third, the above choice ensures that the wave functions of incoming states $|\mathbf{p}\rangle$ and $|\bar{\mathbf{p}}\rangle$ are both e^{-ipx}, i.e., they both oscillate in time with positive frequency like e^{-ip^0t}, thus having a positive energy. With annihilation operators $d_{\mathbf{p}}$ instead of $b^\dagger_{\mathbf{p}}$, the energy of a state created by $d^\dagger_{\mathbf{p}}$ would have been negative. This will also emerge in the calculation of the second-quantized energy to be performed now.

Multiparticle states are formed in the same way as in the real case in Eq. (5.24), except that creation operators $a^\dagger_{\mathbf{p}}$ and $b^\dagger_{\mathbf{p}}$ have to be applied to the vacuum state $|0\rangle$:

$$|n_{\mathbf{p}_1}n_{\mathbf{p}_2}\dots n_{\mathbf{p}_k};\bar{n}_{\mathbf{p}_1}\bar{n}_{\mathbf{p}_2}\dots\bar{n}_{\mathbf{p}_k}\rangle = \mathcal{N}^{S,A}(\hat{a}^\dagger_{\mathbf{p}_1})^{n_{\mathbf{p}_1}}\cdots(\hat{a}^\dagger_{\mathbf{p}_k})^{n_{\mathbf{p}_k}}(b^\dagger_{\mathbf{p}_1})^{\bar{n}_{\mathbf{p}_1}}\cdots(b^\dagger_{\mathbf{p}_k})^{\bar{n}_{\mathbf{p}_k}}|0\rangle. \tag{5.77}$$

As in the real-field case, we shall sometimes use in an infinite volume the single-particle states

$$|\mathbf{p}) = \mathrm{a}^\dagger_{\mathbf{p}}|0), \qquad |\bar{\mathbf{p}}) = \mathrm{b}^\dagger_{\mathbf{p}}|0), \tag{5.78}$$

with the vacuum $|0)$ defined by $\mathrm{a}_{\mathbf{p}}|0) = 0$ and $\mathrm{b}_{\mathbf{p}}|0) = 0$. These states satisfy the same orthogonality relation as the those in (5.26), and have wave functions normalized as in Eq. (5.27).

5.1.5 Energy of Free Charged Scalar Particles

The second-quantized energy density reads

$$\begin{aligned}\mathcal{H}(x) &= \pi(x)\partial^0\phi(x) + \pi^\dagger(x)\partial^0\phi^\dagger(x) - \mathcal{L}(x)\\ &= 2\partial^0\phi^\dagger(x)\partial^0\phi(x) - \mathcal{L}(x)\\ &= \partial^0\phi^\dagger(x)\partial^0\phi(x) + \partial_{\mathbf{x}}\phi^\dagger(x)\partial_{\mathbf{x}}\phi(x) + M^2\phi^\dagger(x)\phi(x).\end{aligned} \tag{5.79}$$

Inserting the expansion (5.72), we find the Hamilton operator [analogous to (5.30)]

$$H = \int d^3x\,\mathcal{H}(x) \;=\; \sum_{\mathbf{p}}\left[\frac{p^{0\,2} + \mathbf{p}^2 + M^2}{2p^0}(a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + b_{\mathbf{p}}b^\dagger_{\mathbf{p}})\right.$$

$$
\begin{aligned}
&\left. + \frac{-p^{0^2} + \mathbf{p}^2 + M^2}{2p^0} \left(a^\dagger_{\mathbf{p}} b^\dagger_{-\mathbf{p}} e^{2ip^0 t} + b_{-\mathbf{p}} a_{\mathbf{p}} e^{-2ip^0 t} \right) \right] \qquad (5.80)\\
&= \sum_{\mathbf{p}} p^0 \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + b^\dagger_{\mathbf{p}} b_{\mathbf{p}} + 1 \right).
\end{aligned}
$$

Note that the mixed terms in the second line appear with opposite momentum labels, since H does not change the total momentum. Had we used $d_{-\mathbf{p}}$ rather than $b^\dagger_{\mathbf{p}}$ in the field expansion, the energy would have been

$$
\begin{aligned}
H = \int d^3x \, \mathcal{H}(x) &= \sum_{\mathbf{p}} \left[\frac{p^{0^2} + \mathbf{p}^2 + M^2}{2p^0} (a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + d^\dagger_{\mathbf{p}} d_{\mathbf{p}}) \right.\\
&\left. + \frac{-p^{0^2} + \mathbf{p}^2 + M^2}{2p^0} (a^\dagger_{\mathbf{p}} d_{\mathbf{p}} e^{2ip^0 t} + d^\dagger_{\mathbf{p}} a_{\mathbf{p}} e^{-2ip^0 t}) \right] \qquad (5.81)\\
&= \sum_{\mathbf{p}} p^0 \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + d^\dagger_{\mathbf{p}} d_{\mathbf{p}} \right).
\end{aligned}
$$

Here the mixed terms have lables with equal momenta. Since the commutation rule of $d_{\mathbf{p}}, d^\dagger_{\mathbf{p}}$ have the wrong sign, the eigenvalues of $d^\dagger_{\mathbf{p}} d_{\mathbf{p}}$ take *negative* integer values implying the energy of the particles created by $d^\dagger_{\mathbf{p}}$ to be negative. For an arbitrary number of such particles, this would imply energies without lower bound, which is unphysical (since it would allow one to build a perpetuum mobile)

Taking the vacuum expectation value of the positive-definite energy (5.80), we obtain as in Eq. (5.31)

$$
E_0 \equiv \langle 0 | H | 0 \rangle = \sum_{\mathbf{p}} p^0 = \sum_{\mathbf{p}} \omega_{\mathbf{p}}, \qquad (5.82)
$$

In comparison with Eq. (5.31), there is a factor 2 since the complex field has twice as many degrees of freedom as a real field. As in the real case, we may subtract this infinite vacuum energy to obtain finite expressions via the earlier explained normal-ordering prescription. Only the gravitational interaction is sensitive to the vacuum energy.

What is the difference between the particle states $|\mathbf{p}\rangle$, $|\bar{\mathbf{p}}\rangle$ created by $a^\dagger_{\mathbf{p}}$ and $b^\dagger_{\mathbf{p}}$? We shall later see that they couple with opposite sign to the electromagnetic field. Here we only observe that they have the same intrinsic properties under the Poincaré group, i.e. the same mass and spin. They are said to be *antiparticles* of each other.

Propagator of Free Charged Scalar Particles

The propagator of the complex scalar field can be calculated in the same fashion as for real fields with the result

$$
\begin{aligned}
G(x, x') &\equiv G(x - x') = \langle 0 | T \phi(x) \phi^\dagger(x') | 0 \rangle\\
&= \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^2 - M^2 + i\eta} e^{-ip(x-x')}. \qquad (5.83)
\end{aligned}
$$

As before, the propagator is equal to the Green function of the free-field equation (5.8). It may again be obtained following the mnemonic rule on p. 282, by Fourier transforming the inverse of the differential operator $L(i\partial)$ in the field equation [recall (5.353) and (5.68)].

5.1.6 Behavior under Discrete Symmetries

Let us now see how the discrete operations of space inversion, time reversal, and complex conjugation of Subsecs 3.5.2–3.5.4 act in the Hilbert space of quantized scalar fields.

Space Inversion

Under a space inversion

$$x' = \tilde{x} = (x_0, -\mathbf{x}), \tag{5.84}$$

a real or complex scalar field is transformed according to

$$\phi(x) \xrightarrow{P} \phi'_P(x) = \eta_P \phi(\tilde{x}), \tag{5.85}$$

with

$$\eta_P = \pm 1. \tag{5.86}$$

For a real field operator $\phi(x)$, this transformation can be achieved by assigning to the creation and annihilation operators $a^\dagger_{\mathbf{p}}, a_{\mathbf{p}}$ in the expansion (5.12) a transformation law

$$\begin{aligned} a'_{\mathbf{p}} &= \eta_P a_{-\mathbf{p}}, \\ a'^\dagger_{\mathbf{p}} &= \eta_P a^\dagger_{-\mathbf{p}}. \end{aligned} \tag{5.87}$$

Indeed, by inserting (5.87) into (5.12) we find

$$\begin{aligned} \phi'_P(x) &= \eta_P \frac{1}{\sqrt{2p^0 V}} \sum_{\mathbf{p}} \left(e^{-ipx} a_{-\mathbf{p}} + e^{ipx} a^\dagger_{-\mathbf{p}} \right) \\ &= \eta_P \frac{1}{\sqrt{2p^0 V}} \sum_{\mathbf{p}} (e^{-ip\tilde{x}} a_{\mathbf{p}} + e^{ip\tilde{x}} a^\dagger_{\mathbf{p}}) = \eta_P \phi(\tilde{x}). \end{aligned} \tag{5.88}$$

It is possible to find a *parity operator* $\mathcal{P}$ in the second-quantized Hilbert space which generates the parity the transformations (5.87), (5.88), i.e., it is defined by

$$\begin{aligned} \mathcal{P} a_{\mathbf{p}} \mathcal{P}^{-1} &\equiv a'_{\mathbf{p}} = \eta_P a_{-\mathbf{p}}, \\ \mathcal{P} a^\dagger_{\mathbf{p}} \mathcal{P}^{-1} &\equiv a'^\dagger_{\mathbf{p}} = \eta_P a^\dagger_{-\mathbf{p}}. \end{aligned} \tag{5.89}$$

An explicit representation of $\mathcal{P}$ is

$$\mathcal{P} = e^{i\pi G_P/2}, \qquad G_P = \sum_{\mathbf{p}} \left[a^\dagger_{-\mathbf{p}} a_{\mathbf{p}} - \eta_P a^\dagger_{\mathbf{p}} a_{\mathbf{p}} \right]. \tag{5.90}$$

In order to prove that this operator has the desired effect, we form the operators

$$a_{\mathbf{p}}^{+\,\dagger} \equiv a_{\mathbf{p}}^{\dagger} + \eta_P\, a_{-\mathbf{p}}^{\dagger}, \qquad a_{\mathbf{p}}^{-\,\dagger} \equiv a_{\mathbf{p}}^{\dagger} - \eta_P\, a_{-\mathbf{p}}^{\dagger}, \tag{5.91}$$

which are invariant under the parity operation (5.89), with eigenvalues ±1:

$$\mathcal{P} a_{\mathbf{p}}^{\pm\,\dagger} \mathcal{P}^{-1} = \pm a_{\mathbf{p}}^{\pm\,\dagger}, \tag{5.92}$$

Then we calculate the same property with the help of the unitary operator (5.90), expanding $e^{iG_P\pi/2} a_{\mathbf{p}}^{\pm\,\dagger} e^{-iG_P\pi/2}$ with the help of Lie's formula (3.99). This turns out to be extremely simple since the first commutators on the right-hand side of (3.99) are

$$[G_P, a_{\mathbf{p}}^{+\,\dagger}] = 0; \qquad [G_P, a_{\mathbf{p}}^{-\,\dagger}] = -2a_{\mathbf{p}}^{-\,\dagger}, \tag{5.93}$$

so that the higher ones are obvious. The Lie series yields therefore

$$\begin{aligned} e^{iG_P\pi/2} a_{\mathbf{p}}^{+\,\dagger} e^{-iG_P\pi/2} &= a_{\mathbf{p}}^{+\,\dagger}, \\ e^{iG_P\pi/2} a_{\mathbf{p}}^{-\,\dagger} e^{-iG_P\pi/2} &= a_{\mathbf{p}}^{-\,\dagger}\left(1 - i\pi + \frac{1}{2!}\pi^2 + \dots\right) = a_{\mathbf{p}}^{-\,\dagger} e^{-i\pi} = -a_{\mathbf{p}}^{-\,\dagger}, \end{aligned} \tag{5.94}$$

showing that the operators $a_{\mathbf{p}}^{\pm\,\dagger}$ do indeed satisfy (5.92).

For a complex field operator $\phi(x)$, the operator G_P in (5.90) has to be extended by the same expression containing the operators $b_{\mathbf{p}}^{\dagger}$ and $b_{\mathbf{p}}$.

Let us denote the multiparticle sates of the type (5.24), (5.77) in the second-quantized Hilbert space collectively by $|\Psi\rangle$. In the Hilbert space of all such states, the operator $\mathcal{P}$ is unitary:

$$\mathcal{P}^{\dagger} = \mathcal{P}^{-1}, \tag{5.95}$$

i.e., for any two states $|\Psi_1\rangle$ and $|\Psi_2\rangle$, the scalar product remains unchanged by $\mathcal{P}$

$${}_P\langle\Psi_1'|\Psi_2'\rangle_P = \langle\Psi_1|\mathcal{P}^{\dagger}\mathcal{P}|\Psi_2\rangle = \langle\Psi_1|\Psi_2\rangle. \tag{5.96}$$

With this operator, the transformation (5.85) is generated by

$$\phi(x) \xrightarrow{P} \mathcal{P}\phi(x)\mathcal{P}^{-1} = \phi'_P(x) = \eta_P \phi(\tilde{x}). \tag{5.97}$$

As an application, consider a state of two identical spinless particles which move in the common center of mass frame with a relative angular momentum l. Such a state is an eigenstate of the parity operation with eigenvalue

$$\eta_P = (-)^l. \tag{5.98}$$

This follows directly by applying the parity operator $\mathcal{P}$ to the wave function

$$|\Psi_{lm}\rangle = \int_0^\infty dp\, R_l(p) \int d^2\hat{\mathbf{p}}\, Y_{lm}(\hat{\mathbf{p}})\, a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger}|0\rangle, \tag{5.99}$$

where $R_l(p)$ is some radial wave function of $p = |\mathbf{p}|$. Using (5.89), the commutativity of the creation operators $a^\dagger_{\mathbf{p}}$ and $a^\dagger_{-\mathbf{p}}$ with each other, and the well-known fact[1] that the spherical harmonic for $-\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}$ differ by a phase factor $(-1)^l$, we find immediately:

$$\mathcal{P}|\Psi_{lm}\rangle = (-1)^l|\Psi_{lm}\rangle. \tag{5.100}$$

For two different bosons of parities η_{P_1} and η_{P_2}, the right-hand side is multiplied by $\eta_{P_1}\eta_{P_2}$.

Time Reversal

The operator implementation of time reversal is not so straightforward. In a time-reversed state all movements are reversed, i.e., for spin zero particles all momenta are reversed (see Subsection 3.5.3). In this respect, there is no difference to the parity operation, and the transformation properties of the creation and annihilation operators are just the same as in (5.89). The associated phase factor is denoted by η_T:

$$\begin{aligned} a'_{\mathbf{p}} &= \eta_T a_{-\mathbf{p}}, \\ a'^\dagger_{\mathbf{p}} &= \eta_T a^\dagger_{-\mathbf{p}}. \end{aligned} \tag{5.101}$$

We have indicated before [see Eq. (3.218)] and shall see below that, in contrast to the phase factor $\eta_P = \pm 1$ of parity, the phase factor η_T will not be restricted to ± 1 by the group structure. It is unmeasurable and can be chosen to be equal to unity,

If we apply the operation (5.101) to the Fourier components in the expansion (5.12) of the field we find

$$\begin{aligned} \phi'_T(x) &= \eta_T \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0V}} \left(e^{-ipx}a_{-\mathbf{p}} + e^{ipx}a^\dagger_{-\mathbf{p}}\right) \\ &= \eta_T \sum_{\mathbf{p}} \frac{1}{\sqrt{2p^0V}} \left(e^{-ip\tilde{x}}a_{\mathbf{p}} + e^{-ip\tilde{x}}a^\dagger_{\mathbf{p}}\right) \\ &= \eta_T \phi(\tilde{x}), \end{aligned} \tag{5.102}$$

which is not yet the correct transformation law (3.198):

$$\phi(x) \xrightarrow{T} \phi'_T(x) = \eta_T \phi(x_T). \tag{5.103}$$

This is achieved by requiring the time reversal transformation to be an *antilinear operator* $\mathcal{T}$ in the multiparticle Hilbert space. It is defined by

$$\begin{aligned} \mathcal{T} a_{\mathbf{p}} \mathcal{T}^{-1} &\equiv a'_{\mathbf{p}} = \eta_T a_{-\mathbf{p}}, \\ \mathcal{T} a^\dagger_{\mathbf{p}} \mathcal{T}^{-1} &\equiv a'^\dagger_{\mathbf{p}} = \eta_T a^\dagger_{-\mathbf{p}}, \end{aligned} \tag{5.104}$$

---

[1] This follows from the property of the spherical harmonic $Y_{lm}(\pi - \theta, \phi) = (-1)^{l-m} Y_{lm}(\theta, \phi)$ together with $e^{im(\phi+\pi)} = (-1)^m e^{im\phi}$.

and by the antilinear property

$$\mathcal{T}(\alpha a+\beta a^\dagger_{\mathbf{p}})\mathcal{T}^{-1}=\alpha^*\mathcal{T}a_{\mathbf{p}}\mathcal{T}^{-1}+\beta^*\mathcal{T}a^\dagger_{\mathbf{p}}\mathcal{T}^{-1}. \tag{5.105}$$

Whenever the time reversal operation is applied to a combination of creation and annihilation operators, the coefficients have to be switched to their complex conjugates. Under this antilinear operation, we indeed obtain (5.103) rather than (5.102):

$$\phi(x)\xrightarrow{T}\mathcal{T}\phi(x)\mathcal{T}^{-1}=\phi'_T(x)=\eta_T\phi(x_T). \tag{5.106}$$

The same transformation law is found for complex scalar fields by defining for particles and antiparticles

$$\begin{aligned}\mathcal{T}a_{\mathbf{p}}\mathcal{T}^{-1}&\equiv a'_{\mathbf{p}}=\eta_T a_{-\mathbf{p}},\\ \mathcal{T}b^\dagger_{\mathbf{p}}\mathcal{T}^{-1}&\equiv b'^\dagger_{\mathbf{p}}=\eta_T b^\dagger_{-\mathbf{p}}.\end{aligned} \tag{5.107}$$

In the second-quantized Hilbert space consisting of states (5.24) and (5.77), the antiunitarity has the consequence that all scalar products are changed into their complex conjugates:

$$\langle\Psi_2|\Psi_1\rangle\xrightarrow{T}{}_T\langle\Psi'_2|\Psi'_1\rangle_T=\langle\Psi_1|\Psi_2\rangle^*, \tag{5.108}$$

thus complying with the property (3.201) of scalar products of ordinary quantum mechanics (to which the second-quantized formalism reduces in the one-particle subspace). This makes the operator $\mathcal{T}$ antiunitary.

To formalize operations with the antiunitary operator $\mathcal{T}$ in the Dirac bra-ket language, it is useful to introduce an antilinear unit operator $\mathbf{1}_A$ which has the effect

$$\langle\Psi_2|\mathbf{1}_A|\Psi_1\rangle\equiv\mathbf{1}_A\langle\Psi_2|\Psi_1\rangle\equiv\langle\Psi_2|\Psi_1\rangle^*. \tag{5.109}$$

The antiunitarity of the time reversal transformation is then expressed by the equation

$$\mathcal{T}^\dagger=\mathcal{T}^{-1}\mathbf{1}_A, \tag{5.110}$$

the operator $\mathbf{1}_A$ causing all differences with respect to the unitary operator (5.95).

Due to the antilinearity, the factor η_T in the transformation law of the complex field is an arbitrary phase factor. We have mentioned this before in Subsec. 3.5.3. By applying the operator $\mathcal{T}$ twice to the complex field $\phi(x)$, we obtain from (5.105)and (5.106):

$$\mathcal{T}^2\phi(x)\mathcal{T}^{-2}=\eta_T\eta_T^*\phi(x), \tag{5.111}$$

so that the cyclic property of time reversal $\mathcal{T}^2=1$ fixes

$$\eta_T\eta_T^*=1. \tag{5.112}$$

This is in contrast to the unitary operators $\mathcal{P}$ and $\mathcal{C}$ where the phases factors must be ±1.

For real scalar fields, this still holds, since the second transformation law (5.104) must be the complex-conjugate of the first, which requires η_T to be real leaving only the choices ±1.

The antilinearity has the consequence that if a Hamilton operator is invariant under time reversal

$$\mathcal{T} H \mathcal{T}^{-1} = H, \tag{5.113}$$

the time evolution operator $U(t,t_0)=e^{-iH(t-t_0)/\hbar}$ satisfies

$$\mathcal{T} U(t,t_0)\mathcal{T}^{-1} = U(t_0,t) = U^\dagger(t,t_0). \tag{5.114}$$

i.e., it has the time order inverted.

The antiunitary nature of $\mathcal{T}$ makes the phase factor η_T of charged fields, an unmeasurable quantity. This why we were able to choose $\eta_T = 1$ after Eq. (5.112) [see also (3.218)] Time reversal invariance does not produce selection rules in the same way as discrete unitary symmetries do, such as parity. This will be discussed in detail in Section 7.7, after having developed the theory of the scattering matrix.

Charge Conjugation

The operator implementation of the transformation (3.219) on a complex scalar field operator

$$\phi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}}\left(e^{-ipx}a_{\mathbf{p}} + e^{ipx}b^\dagger_{\mathbf{p}}\right) \tag{5.115}$$

is quite simple. We merely have to define a *charge conjugation operator* $\mathcal{C}$ by

$$\begin{aligned} \mathcal{C}a^\dagger_{\mathbf{p}}\mathcal{C}^{-1} &= \eta_C b^\dagger_{\mathbf{p}}, & \mathcal{C}b^\dagger_{\mathbf{p}}\mathcal{C}^{-1} &= \eta_C a^\dagger_{\mathbf{p}}, \\ \mathcal{C}a_{\mathbf{p}}\mathcal{C}^{-1} &= \eta_C b_{\mathbf{p}}, & \mathcal{C}b_{\mathbf{p}}\mathcal{C}^{-1} &= \eta_C a_{\mathbf{p}}, \end{aligned} \tag{5.116}$$

where $\eta_C = \pm 1$ is the charge parity of the field, and see that $\mathcal{C}$ produces the desired transformation

$$\phi(x) \xrightarrow{C} \mathcal{C}\phi(x)\mathcal{C}^{-1} = \phi'_C(x) = \eta_C \phi^\dagger(x), \tag{5.117}$$

as in (3.219). For a real field, we may simply identify $b_{\mathbf{p}}$ with $a_{\mathbf{p}}$, thus making the transformation laws (5.116) trivial:

$$\begin{aligned} \mathcal{C}a^\dagger_{\mathbf{p}}\mathcal{C}^{-1} &= \eta_C a^\dagger_{\mathbf{p}}, \\ \mathcal{C}a_{\mathbf{p}}\mathcal{C}^{-1} &= \eta_C a_{\mathbf{p}}, \end{aligned} \tag{5.118}$$

The antiparticles created by $b^\dagger_{\mathbf{p}}$ have the same mass as the particles created by $a^\dagger_{\mathbf{p}}$, but the opposite charge. The latter follows directly from the transformation law (3.221) of the classical local current. In the present second-quantized formulation it is instructive to calculate the matrix elements of the operator current density (3.164),

$$j_\mu(x) = i\varphi^* \overset{\leftrightarrow}{\partial}_\mu \varphi, \tag{5.119}$$

between single-particle states created by $a^\dagger_{\mathbf{p}}$ and $b^\dagger_{\mathbf{p}}$. We find

$$\begin{aligned} \langle \mathbf{p}'|j^\mu(x)|\mathbf{p}\rangle &= \langle 0|a_{\mathbf{p}'}j^\mu(x)a^\dagger_{\mathbf{p}}|0\rangle = (p'^\mu + p^\mu)\frac{1}{\sqrt{2p^0\,2p'^0}}e^{-i(p-p')x}, \\ \langle \bar{\mathbf{p}}'|j^\mu(x)|\bar{\mathbf{p}}\rangle &= \langle 0|b_{\mathbf{p}'}j^\mu(x)b^\dagger_{\mathbf{p}}|0\rangle = -(p'^\mu + p^\mu)\frac{1}{\sqrt{2p^0\,2p'^0}}e^{-i(p-p')x}. \end{aligned} \tag{5.120}$$

The charge of the particle states $|\mathbf{p}\rangle = a^\dagger_{\mathbf{p}}|0\rangle$ and $|\bar{\mathbf{p}}\rangle = b^\dagger_{\mathbf{p}}|0\rangle$ is given by the diagonal matrix element of the charge operator $Q = \int d^3x\, j^0(x)$ between these states.

$$\langle \mathbf{p}'|Q|\mathbf{p}\rangle = \int d^3x \langle \mathbf{p}'|j^0(x)|\mathbf{p}\rangle = \delta_{\mathbf{p}',\mathbf{p}}, \quad \langle \bar{\mathbf{p}}'|Q|\bar{\mathbf{p}}\rangle = \int d^3x \langle \bar{\mathbf{p}}'|j^0(x)|\bar{\mathbf{p}}\rangle = -\delta_{\mathbf{p}',\mathbf{p}}. \tag{5.121}$$

The opposite sign of the charges of particles and antiparticles is caused by the opposite exponentials in the field $\phi(x)$ in (5.115) accompanying the annihilation and creation operators $a_{\mathbf{p}}$ and $b^\dagger_{\mathbf{p}}$, respectively

As far as physical particles are concerned, the states $|\mathbf{p}\rangle = a^\dagger_{\mathbf{p}}|0\rangle$ may be identified with $\pi^\dagger$ mesons of momentum $\mathbf{p}$, the states $|\bar{\mathbf{p}}\rangle = b^\dagger_{\mathbf{p}}|0\rangle$ with $\pi^{(-)}$-mesons. The scalar particles associated with the negative frequency solution of the wave equation are called *antiparticles*. In this nomenclature, the particles of a real field are antiparticles of themselves.

Note that the two matrix elements in (5.120) have the same exponential factors which is necessary for particles and antiparticles to have the same energies and momenta.

An explicit representation of the unitary operator $\mathcal{C}$ is

$$\mathcal{C} = e^{i\pi G_C/2}, \qquad G_C = \sum_{\mathbf{p}} \left[b^\dagger_{\mathbf{p}}a_{\mathbf{p}} + a^\dagger_{\mathbf{p}}b_{\mathbf{p}} - \eta_P(a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + b^\dagger_{\mathbf{p}}b_{\mathbf{p}})\right]. \tag{5.122}$$

The proof is completely analogous to the parity case in Eqs. (5.90)–(5.94).

A bound state of a boson and its antiparticle in a relative angular momentum l has a charge parity $(-1)^l$. This follows directly from the wave function

$$|\Psi\rangle = \int_0^\infty dp\, R_l(p) \int d^2\hat{\mathbf{p}}\, Y_{lm}(\hat{\mathbf{p}})a^\dagger_{\mathbf{p}}b^\dagger_{-\mathbf{p}}|0\rangle, \tag{5.123}$$

where $R_l(p)$ is some radial wave function of $p = |\mathbf{p}|$. Applying $\mathcal{C}$ to this we have

$$\mathcal{C}a^\dagger_{\mathbf{p}}b^\dagger_{-\mathbf{p}}|0\rangle = b^\dagger_{\mathbf{p}}a^\dagger_{-\mathbf{p}}|0\rangle \tag{5.124}$$

and must interchange the order of $b^\dagger_{\mathbf{p}}$ and $a^\dagger_{\mathbf{p}}$, as well as the momenta $\mathbf{p}$ and $-\mathbf{p}$, to get back to the original state. This results in a sign factor $(-1)^l$ from the spherical harmonic. An example is the ρ-meson which is a p-wave resonance of a $\pi^{(+)}$- and a $\pi^{(-)}$-meson, and has therefore a charge parity $\eta_C = -1$.

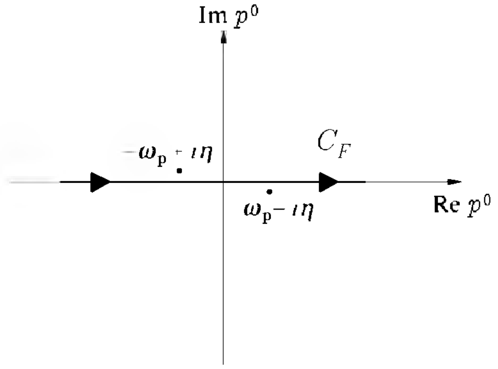

FIGURE 5.1 Pole positions in the complex p^0-plane in the integral representations (5.63) and (5.83) Feynman propagators.

5.2 SPACETIME BEHAVIOR OF PROPAGATORS

Let us evaluate the integral representations (5.63), (5.83) for the propagators of real and complex scalar fields. To do this we use two methods which will be applied many times in this text. The integrand in (5.63), (5.83) has two poles in the complex p^0-plane as shown in Fig. 5.1, one at $p^0 = \sqrt{\mathbf{p}^2 + M^2} - i\eta$, the other at $p^0 = -\sqrt{\mathbf{p}^2 + M^2} + i\eta$ with $\eta > 0$. The first is due to the intermediate single-particle state propagating in the positive time direction, the other to the antiparticle propagating in the negative time direction. A propagator with such pole positions is called a *Feynman propagator*.

5.2.1 Wick Rotation

The special pole positions make it possible to rotate the contour of integration in the p^0-plane without crossing a singularity so that it runs along the imaginary axis $dp^0 = idp^4$. This procedure is called a *Wick rotation*, and is illustrated in Fig. 5.2. Volume elements $d^4p = dp^0dp^1dp^2dp^3$ in Minkowski space go over into volume elements $i\,dp^1dp^2dp^3dp^4 \equiv i\,d^4p_E$ in euclidean space. By this procedure, the integral

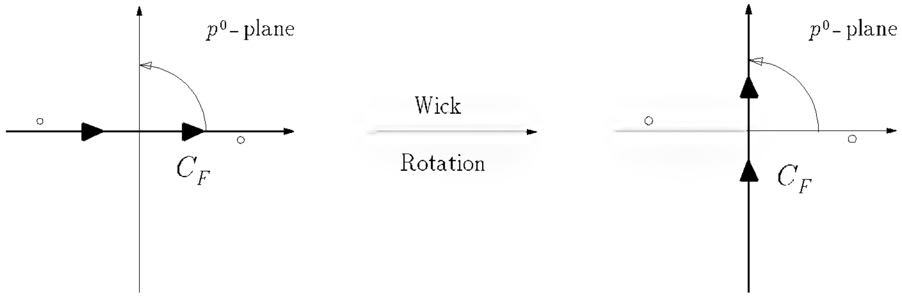

FIGURE 5.2 Wick rotation of the contour of integration in the complex p^0-plane

representations (5.63), (5.83) for the propagator become

$$G(x-x') = \int \frac{d^4p_E}{(2\pi)^4} \frac{1}{p_E^2+M^2} e^{-ip_E(x-x')_E}. \tag{5.125}$$

where p_E^μ is the four-momentum

$$p_E^\mu = (p^1, p^2, p^3, p^4 = -ip^0) \tag{5.126}$$

and p_E^2 the square of the momentum p_E^μ calculated in the euclidean metric, i.e. $p_E^2 \equiv {p^1}^2 + {p^2}^2 + {p^3}^2 + {p^4}^2$. The vector x_E^μ is the corresponding euclidean spacetime vector

$$x_E^\mu = (x^1, x^2, x^3, x^4 = -ix^0), \tag{5.127}$$

so that $px = -p_E x_E$. With $p_E^2 + M^2$ being strictly positive, the integral (5.125) is now well-defined. Moreover, the denominator possesses a simple integral representation in the form of an auxiliary integral over an auxiliary parameter τ which, as we shall see later, plays the role of the *proper time* of the particle orbits:

$$\frac{1}{p_E^2+M^2} = \int_0^\infty d\tau e^{-\tau(p_E^2+M^2)}. \tag{5.128}$$

Since this way of reexpressing denominators in propagators is extremely useful in quantum field theory, it is referred to after its author as *Schwinger's proper-time formalism.*[2] The τ-integral has turned the integral over the denominator into a quadratic exponential function. The exponent can therefore be quadratically completed,

$$e^{ip_E(x-x')_E - \tau p_E^2} \longrightarrow e^{-(x-x')_E^2/4\tau - p'^2\tau}$$

with $p_E' = p_E - i(x-x')_E/2\tau$. Since the measure of integration is translationally invariant, and the integrand has become symmetric under four-dimensional rotations, we can replace

$$\int d^4p_E = \int d^4p_E' = \pi^2 \int_0^\infty dp_E'^2\, p_E'^2, \tag{5.129}$$

and integrate out the four-momentum p_E', yielding

$$G(x-x') = \frac{1}{16\pi^2} \int_0^\infty \frac{d\tau}{\tau^2} e^{-(x-x')_E^2/4\tau - M^2\tau}. \tag{5.130}$$

The integral is a superposition of nonrelativistic propagators of the type (2.393), with Boltzmann-like weights $e^{-M^2\tau}$, and an additonal weight factor τ^{-2} which may be viewed as the effect of an entropy factor $e^S = e^{-2\log\tau}$. This representation has an interesting statistical interpretation. After deriving Eq. (2.393) for a nonrelativistic propagator at imaginary times we observed that this looks like the probability for a random walk of a fixed length proportional to $\hbar\beta$ to go from $\mathbf{x}$ to $\mathbf{x}'$ in three dimensions. Here we see that the relativistic propagator looks like a random walk of arbitrary length in four diemsnions, with a length distribution ruled mainly by the above Boltzmann factor. This leads to the possibility of describing, by relativistic quantum field theory, ensembles of random lines of arbitrary length. Such lines appear in many physical systems in the form of vortex lines and defect lines.[3] Details will be discussed in Chapter 19.

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[2] See Appendix in J. Schwinger, Phys. Rev. *76*, 790 (1949).

By changing the variable of integration from τ to $\omega = 1/4\tau$, this becomes

$$G(x-x') = \frac{1}{4\pi^2}\int_0^\infty d\omega\, e^{-(x-x')_E^2\omega - M^2/4\omega}. \tag{5.131}$$

Now we use the integral formula

$$\int_0^\infty \frac{d\omega}{\omega}\omega^\nu e^{-a\omega-b/4\omega} = 2\left(\frac{b}{4a}\right)^{\nu/2} K_\nu(\sqrt{ab}), \tag{5.132}$$

where $K_\nu(z)$ is the modified Bessel function,[4] we find

$$G(x-x') = \frac{M^2}{4\pi^2}\frac{K_1(M\sqrt{(x-x')_E^2})}{M\sqrt{(x-x')_E^2}}. \tag{5.133}$$

The D-dimensional generalization of this is calculated in the same way. Equation (5.130) becomes

$$G(x-x') = \frac{1}{(4\pi)^{D/2}}\int_0^\infty \frac{d\tau}{\tau^{D/2}} e^{-(x-x')_E^2/4\tau - M^2\tau}, \tag{5.134}$$

yielding via (5.132)

$$\begin{aligned} G(x-x') &= \int \frac{d^Dq}{(2\pi)^D}\frac{1}{q_E^2+M^2}e^{iq(x-x')} \\ &= \frac{1}{(2\pi)^{D/2}}\left(\frac{M}{\sqrt{(x-x')_E^2}}\right)^{D/2-1} K_{D/2-1}(M\sqrt{(x-x')_E^2}). \end{aligned} \tag{5.135}$$

5.2.2 Feynman Propagator in Minkowski Space

Let us now do the calculation in Minkowski space. There the a proper-time representation of the propagator (5.63), (5.83) reads

$$G(x-x') = \int \frac{d^4p}{(2\pi)^4}\frac{i}{p^2-M^2+i\eta}e^{-ip(x-x')} = \int_0^\infty d\tau \int \frac{d^4p}{(2\pi)^4} e^{-i[p(x-x')-\tau(p^2-M^2+i\eta)]}. \tag{5.136}$$

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[3] See the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, World Scientific, 1989 (http://www.physik.fu-berlin.de/~kleinert/kleiner_re.html#b1), and H. Kleinert, *Proceedings of a NATO Advanced Study Institute on Formation and Interactions of Topological Defects* at the University of Cambridge, England (cond-mat/9503030).

[4] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 3.471.9.

The momentum integrations can be done, after a quadratic completion, with the help of Fresnel's formulas

$$\int \frac{dp^0}{2\pi} e^{ip^{0\,2}a} = \frac{1}{2\sqrt{\pi a/i}}, \qquad \int \frac{dp^i}{2\pi} e^{ip^{i\,2}a} = \frac{1}{2\sqrt{\pi a/i}}. \tag{5.137}$$

In these, it does not matter (as it did before in the Gauss integrals) that $p^{0\,2}$ and $p^{i\,2}$ appear with opposite signs in the exponent.

In continuing the evaluation of (5.136) it is necessary to make sure that the integrals over dp^μ and $d\tau$ can be interchanged. The quadratic completion generates a term $e^{-i(x-x')^2/4\tau}$ which is integrable for $\tau \to 0$ only if we replace $(x-x')^2$ by $(x-x')^2 - i\eta$. Changing again τ to $\omega = 1/4\tau$ we arrive at the integral representation for the Feynman propagator

$$G(x-x') = -\frac{i}{4\pi^2}\int_0^\infty d\omega\, e^{-i\{[(x-x')^2-i\eta]\omega+(M^2-i\eta)/4\omega\}}. \tag{5.138}$$

The two small imaginary parts are necessary to make the integral convergent at both ends. The integral can be done with the help of the formula[5]

$$\int_0^\infty \frac{d\omega}{\omega}\omega^\nu e^{i(a\omega+b/4\omega)} = 2\left(\frac{b}{4a}\right)^{\nu/2} i\frac{\pi}{2}e^{i\pi\nu/2}H_\nu^{(1)}(\sqrt{ab}), \tag{5.139}$$

where $H_\nu^{(1)}(z)$ is the Hankel function of the first kind. Upon taking the complex conjugate, using[6]

$$[H_\nu^{(1)}(z)]^* = H_\nu^{(2)}(z^*), \tag{5.140}$$

and replacing a by a^* and b by b^*, we obtain

$$G(x-x') = i\frac{M^2}{8\pi}\frac{H_1^{(2)}(M\sqrt{(x-x')^2})}{M\sqrt{(x-x')^2}}. \tag{5.141}$$

The Hankel functions are combinations of Bessel and Neumann functions

$$H_\nu^{(1,2)}(z) = J_\nu(z) \pm iN_\nu(z). \tag{5.142}$$

In order to check the correctness of this expression, we go to the nonrelativistic limit by letting $c \to \infty$ in the argument of the Hankel function. Displaying the true cgs units, for clarity, this becomes

$$\frac{M}{\hbar}\sqrt{(x-x')^2} = \frac{M}{\hbar}\sqrt{c^2(t-t')^2 - (\mathbf{x}-\mathbf{x}')^2} \approx \frac{Mc^2\,(t-t')}{\hbar} - \frac{1}{2}\frac{M}{\hbar}\frac{(\mathbf{x}-\mathbf{x}')^2}{2(t-t')}. \tag{5.143}$$

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[5] ibid., Formula 3.471.11, together with 8.476.9.

[6] The last two identities are from ibid., Formulas 8.476.8 and 8.476.11.

For large arguments, the Hankel functions behave like

$$H_\nu^{(1,2)}(z) \approx \frac{2}{\pi z} e^{\pm i(z-\nu\pi/2-\pi/2)}, \tag{5.144}$$

so that (5.141) becomes for $t > t'$, taking account the nonrelativistic limit (3.151) of the fields,

$$G(x-x') \xrightarrow{c\to\infty} \frac{1}{2M} \frac{1}{\sqrt{2\pi i\hbar(t-t')/M}^3} \exp\left[\frac{i}{\hbar}\frac{M}{2t}(\mathbf{x}-\mathbf{x}')^2\right]. \tag{5.145}$$

in agreement with the nonrelativistic propagator (2.243).

In the spacelike regime $(x-x')^2 < 0$, we continue $\sqrt{(x-x')^2}$ to $-i\sqrt{-(x-x')^2}$, and $H_1^{(2)}(z) = H_1^{(1)}(-z)$ together with the relation[7]

$$\frac{\pi i}{2} \frac{H_\nu^{(1)}(iz)}{(iz)^\nu} = \frac{K_\nu(z)}{z^\nu} \tag{5.146}$$

to rewrite (5.141) as

$$G(x-x') = \frac{M}{4\pi^2} \frac{K_1(M\sqrt{-(x-x')^2})}{M\sqrt{-(x-x')^2}}, \qquad (x-x')^2 < 0. \tag{5.147}$$

in agreement with (5.133).

It is instructive to study the massless limit $M \to 0$, in which the asymptotic behavior[8] $K(z) \to 1/z$ leads to

$$G(x-x') \to \frac{1}{4\pi^2} \frac{1}{(x-x')_E^2}. \tag{5.148}$$

To continue this back to Minkowski space where $(x-x')_E^2 = -(x-x')^2$, it is necessary to remember the small negative imaginary part on x^2 which was necessary to make the τ-integral (5.138) converge. The correct massless Green function in Minkowski space is therefore

$$G(x-x') = -\frac{1}{4\pi^2} \frac{1}{(x-x')^2 - i\eta}. \tag{5.149}$$

The same result is obtained form the $M \to 0$ -limit of the Minkowski space expression (5.141), using the limiting property[9]

$$H_\nu^{(1)}(z) \approx -H_\nu^{(2)}(z) \approx -\frac{i}{\pi}\Gamma(\nu)\frac{1}{(z/2)^\nu}. \tag{5.150}$$

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[7] ibid., Formula 8.407.1.

[8] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Formula 9.6.9.

[9] ibid., Formula 9.1.9.

5.2.3 Retarded and Advanced Propagators

Let us contrast the spacetime behavior of the Feynman propagators (5.141) and (5.149) from that of the *retarded propagator* of classical electrodynamics. A retarded propagator is defined for an arbitrary interacting field $\phi(x)$ by the expectation value

$$G_R(x-x') \equiv \Theta(x^0-x'^0)\langle 0|[\phi(x),\phi(x')]|0\rangle. \tag{5.151}$$

In general, one defines a commutator function $C(x-x')$ by

$$C(x-x') \equiv \langle 0|[\phi(x),\phi(x')]|0\rangle, \tag{5.152}$$

and has the relation

$$G_R(x-x') = \Theta(x^0-x'^0)C(x-x'), \tag{5.153}$$

For a free field $\phi(x)$, the commutator is a c-number, so that the vacuum expectation values can be omitted, and $C(x-x')$ is given by (5.53), leading to a retarded propagator

$$G_R(x-x') = \Theta(x^0-x'^0)[G^{(+)}(x-x')-G^{(-)}(x-x')], \tag{5.154}$$

The Heaviside function in front of the commutator function $C(x-x')$ ensures the causality of this propagator. It also has the effect of changing $C(x-x')$ which solves the homogenous Klein-Gordon equation into a solution of the inhomogenoous equation. In fact, by comparing the (5.154) with (5.59) and using the Fourier representations (5.60) of the Heaviside functions, we find for the retarded propagator a representation very similar to that of the Feynman propagator in (5.61), except that the $i\eta$ in the negative-energy pole term is reversed:

$$G_R(x-x') = \int \frac{dE}{2\pi}\frac{d^3p}{(2\pi)^3}\frac{1}{2p^0}\left(\frac{i}{E-p^0+i\eta}-\frac{i}{E+p^0+i\eta}\right)e^{-iE(x_0-x'_0)+i\mathbf{p}(\mathbf{x}-\mathbf{x}')}, \tag{5.155}$$

By combining the denominators we now find, instead of (5.62),

$$\int \frac{dE}{2\pi}\frac{d^3p}{(2\pi)^3}\frac{i}{(E+i\eta)^2-\mathbf{p}^2-M^2}e^{-iE(x_0-x'_0)+i\mathbf{p}(\mathbf{x}-\mathbf{x}')}, \tag{5.156}$$

which may be written as an off-shell integral as in (5.63):

$$G_R(x-x') = \int \frac{d^4p}{(2\pi)^4}\frac{i}{p_+^2-M^2+i\eta}e^{-ip(x-x')}, \tag{5.157}$$

where the subscript of p_+ indicates that a small term $i\eta$ has been added to p^0.

Note the difference in the Fourier representation with respect to that of the commutator function in (5.56), which solves the homogenous Klein-Gordon equation.

It is important to realize that the retarded Green function could be derived from a time-ordered expectation value of second-quantized field operators if the Fourier components of the negative frequencies were associated with annihilation operators $d_{-\mathbf{p}}$ rather than creation operators $b^\dagger_{\mathbf{p}}$ of antiparticles. Then the propagator would vanish for $x^0 < x'^0$, implying both poles in the p^0-plane to lie below the real energy axis.

For symmetry reasons, one also introduces an advanced propagator

$$G_A(x-x') \equiv \Theta(x'^0 - x^0)\langle 0|[\phi(x), \phi(x')]|0\rangle. \tag{5.158}$$

It has the same Fourier representation as $G_R(x-x')$, except that the poles lie both above the real axis:

$$G_A(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p_-^2 - M^2} e^{-ip(x-x')}. \tag{5.159}$$

There will be an application of this Green function in Subsec. ??.

Let us calculate the spacetime behavior of the retarded propagator in spacetime. We shall fist look at the massless case familiar from classical electrodynamics. For $M = 0$, the integral representation (5.157) reads

$$G_R(x-x') \equiv \int \frac{d^4p}{(2\pi)^4} e^{-ip(x-x')} \frac{i}{p_+^2}, \tag{5.160}$$

but with the poles in the p^0-plane at

$$p^0 = p^0 = \pm\omega_{\mathbf{p}} = \pm|\mathbf{p}|. \tag{5.161}$$

both placed *below* the real axis. This is indicated by writing p_+^2 in the denominator rather than p^2, the plus sign indicating an infinitesimal $+i\eta$ added to p^0.

In the Feynman case, the p^0-integral is evaluated with the decomposition (5.61) and the integral representation (5.60) of the Heaviside function] as follows:

$$\begin{aligned} &\int \frac{dp^0}{2\pi} e^{-ip^0(x^0-x'^0)} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{1}{p^0 - \omega_{\mathbf{p}} + i\eta} - \frac{1}{p^0 + \omega_{\mathbf{p}} - i\eta} \right) \\ &\quad = \frac{1}{2\omega_{\mathbf{p}}} [\Theta(x^0 - x'^0) e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} + \Theta(x'^0 - x^0) e^{i\omega_{\mathbf{p}}(x^0-x'^0)}] = \frac{1}{2\omega_{\mathbf{p}}} e^{-i\omega_{\mathbf{p}}|x^0-x'^0|}. \end{aligned} \tag{5.162}$$

In contrast, the retarded expression reads

$$\begin{aligned} &\int \frac{dp^0}{2\pi} e^{-ip^0(x^0-x'^0)} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{1}{p^0 - \omega_{\mathbf{p}} + i\eta} - \frac{1}{p^0 + \omega_{\mathbf{p}} + i\eta} \right) \\ &\qquad\qquad = \Theta(x^0 - x'^0) \frac{1}{2\omega_{\mathbf{p}}} [e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} - e^{i\omega_{\mathbf{p}}(x^0-x'^0)}]. \end{aligned} \tag{5.163}$$

Thus we may write

$$\begin{aligned} G(x-x') &= \int \frac{d^3p}{(2\pi)^3 2\omega_{\mathbf{p}}} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} e^{-i\omega_{\mathbf{p}}|x^0-x'^0|}, & (5.164) \\ G_R(x-x') &= \Theta(x^0 - x'^0) \int \frac{d^3p}{(2\pi)^3 2\omega_{\mathbf{p}}} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} [e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} - e^{i\omega_{\mathbf{p}}(x^0-x'^0)}]. & (5.165) \end{aligned}$$

In the retarded expression we recognize, after the factor $\Theta(x^0 - x'^0)$, the massless limit of the commutator function $C(x, x') = C(x - x')$ of Eq. (5.54), in accordance with the general relation (5.153).

The angular parts of the spatial part of the Fourier integral

$$\int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \tag{5.166}$$

are the same in both cases, producing an integral over $|\mathbf{p}|$:

$$\frac{1}{2\pi R}\int_0^\infty \frac{d|\mathbf{p}|}{\pi}\, |\mathbf{p}| \,\sin\, |\mathbf{p}|R, \tag{5.167}$$

where $R \equiv |\mathbf{x} - \mathbf{x}'|$. The Feynman propagator has therefore integral representation

$$G(x - x') \;=\; \frac{1}{4\pi R}\int_0^\infty \frac{d|\mathbf{p}|}{\pi}\frac{|\mathbf{p}|}{\omega_{\mathbf{p}}} \sin\, |\mathbf{p}|R\, e^{-i\omega_{\mathbf{p}}|x^0-x'^0|}. \tag{5.168}$$

In the massless case where $\omega_{\mathbf{p}} = |\mathbf{p}|$, we can easily perform the $|\mathbf{p}|$-integration and recover the previous result (5.149).

To calculate the retarded propagator $G_R(x - x') = \Theta(x^0 - x'^0)\, C(x - x')$ in spacetime, we may focus our attention upon the commutator function, whose integral representation is now

$$C(x - x') = \frac{1}{4\pi R}\int_0^\infty \frac{dp}{\pi}\frac{p}{\omega_{\mathbf{p}}} \sin\, pR\, [e^{-i\omega_{\mathbf{p}}(x^0-x'^0)} - e^{i\omega_{\mathbf{p}}(x^0-x'^0)}]. \tag{5.169}$$

In the massless case where $\omega_{\mathbf{p}} = p$, we decompose the trigonometric function into exponentials, and obtain

$$C(x - x') = -i\frac{1}{4\pi R}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\left\{e^{-i\omega[(x^0-x'^0)-R]} - e^{-i\omega[(x^0-x'^0)+R]}\right\}, \tag{5.170}$$

which is equal to

$$C(x - x') = -i\frac{1}{4\pi R}\left[\delta(x^0 - x'^0 - R) - \delta(x^0 - x'^0 + R)\right]. \tag{5.171}$$

It is instructive to verify in this expression the canonical equal-time commutation properties (5.55). For this we multiply $\dot{C}(x)$ by a test function $f(r)$ and calculate, with $r = |\mathbf{x}|$,

$$\int d^3x\, \dot{C}(x) f(r) = -i\int dr\, r^2\frac{1}{r}\left[\dot\delta(x^0 - r) - \dot\delta(x^0 + r)\right] = \tag{5.172}$$

Since $\dot\delta(x^0 - r) - \dot\delta(x^0 + r) = -(d/dr)[\delta'(x^0 - r) + \delta'(x^0 + r)]$, we can perform a partial integration and find

$$-\, i\int dr\, \left[\delta(x^0 - r) + \dot\delta(x^0 + r)\right] [rf(r)]' = -i\frac{d}{dx^0}[|x^0| f(|x^0|)]. \tag{5.173}$$

At $x^0=0$, this is equal to $-if(0)$ at $x^0=0$, as it should.

Using the property of the δ-function (5.58) in spacetime

$$\delta(x^{02}-r^2)=\frac{1}{2r}[\delta(x^0-r)+\delta(x^0+r)]. \tag{5.174}$$

we can write the commutator function also as

$$C(x-x')=-i\epsilon(x^0-x'^0)\,\frac{1}{2\pi}\delta((x-x')^2). \tag{5.175}$$

where $\epsilon(x^0-x'^0)$ is defined by

$$\epsilon(x^0-x'^0)\equiv\Theta(x^0-x'^0)-\Theta(-x^0+x'^0), \tag{5.176}$$

which changes the sign of the second term in the decomposition (5.174) of $\delta((x-x')^2)$ to the form required in (5.174).

Note that in the form (5.175), the canonical properties (5.55) of the commutator function cannot directly be verified since $\dot\epsilon(x^0-x'^0)=2\delta(x^0-x'^0)$ is too singular to be evaluated at equal times. In fact, products of distributions are in general undefined, and their use is forbidden in mathematics.[10] We must read $\epsilon(x^0)\delta(x^2)$ as the single distribution

$$\epsilon(x^0)\delta(x^2)\equiv\frac{1}{2r}[\delta(x^0-r)-\delta(x^0+r)] \tag{5.177}$$

which it represents to deduce its properties.

With (5.171) and (5.175), the retarded propagator becomes [recall (5.153)]

$$\begin{aligned}G_R(x-x') &= -i\Theta(x^0-x'^0)\frac{1}{4\pi R}\left[\delta(x^0-x'^0-R)-\delta(x^0-x'^0+R)\right]\\ &= -i\Theta(x^0-x'^0)\,\frac{1}{2\pi}\delta((x-x')^2).\end{aligned} \tag{5.178}$$

The Heaviside function allows only positive $x^0-x'^0$, so that only the first δ-function in (5.178) contributes, and we obtain the well-known expression of classical electrodynamics

$$G_R(x-x')=-i\Theta(x^0-x'^0)\frac{1}{4\pi R}\delta(x^0-x'^0-R). \tag{5.179}$$

This propagator exists only for a causal time order $x^0>x'^0$, for which it is equal to the Coulomb potential between points which can be connected by a light signal.

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[10] See, however, the recent extension of distribution theory to include products in the textbook H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* World Scientific, Singapore 2002, third extended edition (`http://www.physik.fu-berlin.de/~kleinert/re.html#b7`).

The retarded propagator $G_R(x, x')$ describes the massless scalar field $\phi(x)$ caused by a local spacetime event $i\delta^{(4)}(x')$. For a general source $j(x')$, it serves to solve the inhomogeneous field equation

$$-\partial^2\phi(x) = j(x) \tag{5.180}$$

by superposition:

$$\phi(x) = -i\int d^4x\, G_R(x, x')j(x'). \tag{5.181}$$

Inserting (5.179) and separating the integral into time and space parts, the time x_0' can be integrated out and the result becomes

$$\phi(\mathbf{x}, t) = -\int d^3x' \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}j(\mathbf{x}', t_R), \tag{5.182}$$

where

$$t_R = t - |\mathbf{x}-\mathbf{x}'| \tag{5.183}$$

is the time at which the source has emitted the field which arrives at the spacetime point x. Relation (5.182) is the basis for the derivation of the *Liénard-Wiechert potential*, which is recapitulated in Appendix 5A.

5.2.4 Comparison of Singular Functions

Let us compare the spacetime behavior (5.178), (5.179) of the retarded propagator with that of the massless Feynman propagator. The denominator in (5.149) can be decomposed into partial fractions, and we find a form very close to (5.178):

$$G(x-x') = -\frac{1}{8\pi^2 R}\left[\frac{1}{|x^0 - x'^0| - R - i\eta} - \frac{1}{|x^0 - x'^0| + R - i\eta}\right]. \tag{5.184}$$

Feynman has found it useful to denote the function $1/(t - i\eta)$ by $i\pi\delta_+(t)$. This has a Fourier representation which differs from that of a Dirac δ-function by containing only positive frequencies:

$$\delta_+(t) \equiv \int_0^\infty \frac{d\omega}{\pi} e^{-i\omega(t-i\eta)}. \tag{5.185}$$

The integral converges at large frequencies only due to the $-i\eta$ -term, yielding

$$\delta_+(t) = -\frac{1}{\pi}\frac{i}{t-i\eta}. \tag{5.186}$$

The pole term can be decomposed as

$$\frac{1}{t-i\eta} = \frac{i\eta}{t^2+\eta^2} + \frac{t}{t^2+\eta^2} = i\pi\delta(t) + \frac{\mathcal{P}}{t}, \tag{5.187}$$

Recall that the decomposition concerns distributions which make sense only if they are used inside integrals as multiplyers of smooth functions. The symbol $\mathcal{P}$ in the second term means that the integral has to be calculated with the *principal-value* prescription.[11] For the function $\delta_+(t)$, the decomposition reads

$$\delta_+(t) = \delta(t) - \frac{i}{\pi}\frac{\mathcal{P}}{t}. \tag{5.188}$$

An important property of this function is that it satisfies a relation like $\delta(t)$ in (5.174):

$$\delta_+(t^2 - r^2) = \frac{1}{2r}[\delta_+(t-r) - \delta_+(t+r)]. \tag{5.189}$$

Below we shall also need the complex conjugate of the function $\delta_+(t)$:

$$\delta_-(t) = \frac{1}{\pi}\frac{i}{t+i\eta} = [\delta_+(t)]^*. \tag{5.190}$$

From (5.187) we see that the two functions are related by

$$\delta_+(t) + \delta_-(t) = 2\delta(t). \tag{5.191}$$

Because of (5.189), the Feynman propagator (5.184) can be rewritten as

$$G(x-x') = -\frac{1}{8\pi^2 R}\Big[\delta_+(|x^0 - x'^0| - R) - \delta_+(|x^0 - x'^0| + R)\Big] = -\frac{i}{4\pi}\delta_+((x-x')^2). \tag{5.192}$$

These expressions look very similar to those for the retarded propagator in Eqs. (5.178) and Eqs. (5.179).

It is instructive to see what becomes of the δ_+-function in Feynman propagators in the presence of a particle mass. According to (5.138), a mass term modifies the integrand in

$$\delta_+((x-x')^2) = \int_0^\infty \frac{d\omega}{\pi} e^{-i\omega(x-x')^2}, \tag{5.193}$$

(in which we omit the $-i\eta$ term, for brevity) from $e^{-i\omega(x-x')^2}$ to $e^{-i\omega(x-x')^2 - iM^2/4\omega}$. We may therefore define a massive version of $\delta_+((x-x')^2)$ by

$$\delta_+^M((x-x')^2) = \int_0^\infty \frac{d\omega}{\pi} e^{-i\omega(x-x')^2 - iM^2/2\omega} = -\frac{M^2}{2}\frac{H_1^{(2)}(M\sqrt{(x-x')^2})}{M\sqrt{(x-x')^2}}. \tag{5.194}$$

A similar generalization of the function $\delta((x-x')^2)$ in (5.175) to $\delta^M((x-x')^2)$ may be found by evaluating the commutator function $C(x-x')$ in Eq. (5.175) at a nonzero mass M. Its Fourier representation was given in Eq. (5.169) and may be written as

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[11] Because of the entirely different contexts, no confusion is possible with the second-quantized parity operator $\mathcal{P}$ introduced in (5.89).

$$C(x-x') = -\frac{i}{2\pi^2}\int_0^\infty \frac{d|\mathbf{p}|\,|\mathbf{p}|^2}{\sqrt{|\mathbf{p}|^2+M^2}}\frac{\sin|\mathbf{p}|r}{|\mathbf{p}|r}\sin p^0(x^0-x'^0) \qquad (5.195)$$

This can be expressed as a derivative

$$C(x-x') = -\frac{i}{4\pi}\frac{1}{r}\frac{d}{dr}F(r,x^0-x'^0) \qquad (5.196)$$

of the function

$$F(r,t) \;=\; \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{dp}{\sqrt{p^2+M^2}}\cos pr\,\sin\sqrt{p^2+M^2}t \qquad (5.197)$$

The integral yields[12]

$$F(r,t) = \begin{cases} J_0(M\sqrt{t^2-r^2}) & \text{for} \quad t>r, \\ 0 & \text{for} \quad t\in(-r,r), \\ -J_0(M\sqrt{t^2-r^2}) & \text{for} \quad t<-r, \end{cases} \qquad (5.198)$$

where $J_\mu(z)$ are Bessel functions. By carrying out the differentiation in (5.196) using $J_0'(z) = -J_1(z)$, we may write

$$C(x-x') = -i\epsilon(x^0-x'^0)\delta^M((x-x')^2), \qquad (5.199)$$

with

$$\delta^M(x^2) = \delta(x^2) - \Theta(x^2)\frac{M^2}{2}\frac{J_1(M\sqrt{x^2})}{M\sqrt{x^2}}. \qquad (5.200)$$

The function $\Theta(x^2)$ enforces the vanishing of the commutator at spacelike distances, a necessity for the causality of the theory. Using (5.200), we can write the retarded propagator $G_R(x-x') = \Theta(x^0-x'^0)\,C(x-x')$ as

$$G_R(x-x') = -i\Theta(x^0-x'^0)\frac{1}{2\pi}\delta^M((x-x')^2). \qquad (5.201)$$

In the massless limit, the second term in (5.200) disappears since $J_1(z) \approx z$ for small z, and (5.201) reduces to (5.178).

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[12] See Appendix in J. Schwinger, Phys. Rev. *75*, 651 (1949); also ibid. *76*, 790 (1949); *82*, 664, 914 (1951); *91*, 713, 728 (1953); *92*, 1283 (1953); *93*, 615 (1954); *Quantum Electrodynamics*, Dover, New York, 1958.

Summarizing, we may list the Fourier transforms of the various propagators as follows:

$$
\begin{aligned}
\text{Feynman propagator :}\quad & \frac{i}{p^2-M^2+i\eta} = \pi\delta_-(p^2-M^2) = \pi\delta_-(p^{02}-\omega_{\mathbf{p}}^2),\\
& \qquad\qquad = \frac{\pi}{2\omega_{\mathbf{p}}}[\delta_-(p^0-\omega_{\mathbf{p}})+\delta_+(p^0+\omega_{\mathbf{p}})],\\
\text{retarded propagator :}\quad & \frac{i}{p_+^2-M^2} = \frac{\pi}{2\omega_{\mathbf{p}}}[\delta_-(p^0-\omega_{\mathbf{p}})-\delta_-(p^0+\omega_{\mathbf{p}})],\\
\text{advanced propagator :}\quad & \frac{i}{p_-^2-M^2} = -\frac{\pi}{2\omega_{\mathbf{p}}}[\delta_+(p^0-\omega_{\mathbf{p}})-\delta_+(p^0+\omega_{\mathbf{p}})],\\
\text{commutator :}\quad & 2\pi\epsilon(p^0)\delta(p^2-M^2) = 2\pi\epsilon(p^0)\delta(p^{02}-\omega_{\mathbf{p}}^2)\\
& \qquad\qquad = \frac{\pi}{\omega_{\mathbf{p}}}[\delta_-(p^0-\omega_{\mathbf{p}})-\delta_+(p^0+\omega_{\mathbf{p}})],
\end{aligned}
\tag{5.202}
$$

The corresponding integration contours in the complex energy plane of the representations of the spacetime propagators are indicated in Fig. 5.3.

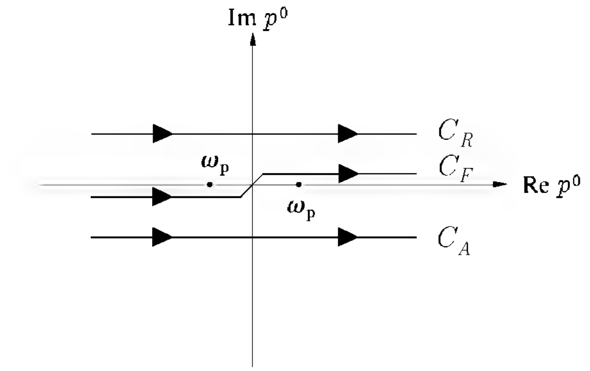

FIGURE 5.3 Integration contours in the complex p^0-plane of the Fourier integral for the various propagators: C_F for the Feynman propagator, C_R for the retarded and C_A for the advanced propagators.

A little exercise with these functions, is given in Appendix 5B.

We end this section by pointing out an important physical property of the euclidean Feynman propagator. When generalizing its proper-time representation to D spacetime dimensions, it reads

$$
G(x-x') = \int_0^\infty d\tau \frac{1}{\sqrt{4\pi\tau}^D} e^{-(x-x')_E^2/4\tau - M^2\tau}. \tag{5.203}
$$

reducing to (5.130) for $D=4$. The integrand can be interpreted as the probability[13] that a random world line of length $L = 2D\tau/a$ which is stiff over a length scale

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[13] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics,*, World Scientific Publishing Co., Singapore 1995, Second extended edition, Sections 5.84 and 15.7.

$a = 2D$, and has the end-to-end distance $x - x'$. Thus the Feynman propagator gives then the probability of a particle worldline connecting via all possible random shapes the points x and x'. Each line is weighted with a Boltzmann probability $e^{-M^2\tau}$ depending on the various lengths. In recent years this observation has been very fruitful by giving rise to a new type of quantum field theory, the so-called *disorder field theories.*[14] They permit us to study phase transitions of a variety of different physical systems in a uniform way that is dual to Landau's famous theory. These transitions have in common that they can be interpreted as a consequence of a sudden proliferation of line-like excitations, caused by an overwhelming configuration entropy. The proliferation occurs at a temperature at which the configurational entropy outweighs the Boltzmann suppression, the latter being proportional to the length of the line-like excitations.

Examples are polymers in solutions, vortex lines in superfluids, and defect lines in crystals. Whereas the traditional field theoretic description of phase transitions due to Landau is based on the introduction of an *order parameter* and its spacetime version, an *order field*, the new description is based on a *disorder field* describing random fluctuations of line-like excitations. As a result of this different way of looking at phase transitions one obtains a field theoretic formulation of the statistical mechanics of line ensembles, and based on it a simple explanation of the phase transitions in superfluids and solids.

5.3 FREE DIRAC FIELDS

We now turn to the quantization of the Dirac field obeying the field equation (3.454):

$$(i\gamma^\mu \partial_\mu - M)\psi(x) = 0. \tag{5.204}$$

Their plane-wave solutions were given in Subsec. 3.14.1, and just as in the case of a scalar field, we shall introduce creation and annihiation operators for particles associated with these solutions.

The classical Lagrangian density is [recall (3.455)]:

$$\mathcal{L}(x) = \bar\psi(x) i\gamma^\mu \partial_\mu \psi(x) - M\bar\psi(x)\psi(x). \tag{5.205}$$

5.3.1 Field Quantization

The canonical momentum of the $\psi(x)$ field is

$$\pi(x) = \frac{\partial\mathcal{L}(x)}{\partial[\partial^0\psi(x)]} = i\bar\psi(x)\gamma^0 = i\psi^\dagger(x). \tag{5.206}$$

---

[14] H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I Superflow and Vortex Lines, Vol. II Stresses and Defects, World Scientific, Singapore 1989.

Up to the factor i, this is equal to the complex-conjugate field $\psi^\dagger$, as in the nonrelativistic equation (5.4.1). As there, the field $\bar{\psi}$ has no conjugate momentum, since

$$\frac{\partial \mathcal{L}(x)}{\partial[\partial^0 \bar{\psi}(x)]} = 0. \tag{5.207}$$

This is again a mere artifact of the use of complex field variables and unrelated to a more severe problem in Section 5.4.1, where the canonical momentum of a component of the real electromagnetic vector field vanishes as a consequence of gauge invariance.

If $\psi(\mathbf{x}, t)$ were a Bose field, its canonical commutation rule would read

$$[\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)] = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{5.208}$$

However, since electrons must obey Fermi statistics to produce the periodic system of elements, the fields have to satisfy anticommutation rules

$$\left\{\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t)\right\} = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{5.209}$$

Whereas in the nonrelativistic case, this modifications of the commutation rules was dictated by the Pauli principle and the implied antisymmetric electronic wave functions, the relativistic theory can only be quantized by anticommutation rules, and commutation rules (5.208) are incompatible either with microcausality or the positivity of the energy. This will be shown in Section 5.8.

We now expand the field $\psi(x)$ into the complete set of classical plane-wave solutions (3.601) in a large but finite volume V:

$$\psi(x) = \sum_{\mathbf{p}, s_3} \left[f_{\mathbf{p}\, s_3}(x) a_{\mathbf{p}, s_3} + f^c_{\mathbf{p}\, s_3}(x) b^\dagger_{\mathbf{p}, s_3} \right], \tag{5.210}$$

or explicitly:

$$\psi(x) = \sum_{\mathbf{p}, s_3} \frac{1}{\sqrt{V p^0/M}} \left[e^{-ipx} u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ipx} v(\mathbf{p}, s_3) b^\dagger_{\mathbf{p}, s_3} \right]. \tag{5.211}$$

As in the scalar equation (5.12) we have associated the expansion coefficients of the plane waves e^{ipx} with a creation operator $b^\dagger_{\mathbf{p}, s_3}$ rather than an annihilation operator. one $d^\dagger_{-\mathbf{p}, -s_3}$. for quite similar reasons [recall the discussion after Eqs. (5.72) and (5.80)]. The reason a sign reversal of s_3 is similar to that for the momentum, and will be expained below.

Expansion (5.211) is inverted and solved for $a_{\mathbf{p}, s_3}$ and $b^\dagger_{\mathbf{p}, s_3}$ by applying the orthogonality relations (3.604) for the bispinors $u(\mathbf{p}, s_3)$ and $v(-\mathbf{p}, s_3)$ to the spatial Fourier transform

$$\int d^3x\, e^{-i\mathbf{p}\mathbf{x}} \psi(x) = \sum_{\mathbf{p}, s_3} \frac{\sqrt{V}}{\sqrt{p^0/M}} \left[e^{-ip^0x^0} u(\mathbf{p}, s_3) a_{\mathbf{p}, s_3} + e^{ip^0x^0} v(-\mathbf{p}, s_3) b^\dagger_{-\mathbf{p}, s_3} \right] \tag{5.212}$$

The result is

$$\begin{aligned} a_{\mathbf{p},s_3} &= e^{ip^0x^0}\,\frac{1}{\sqrt{Vp^0/M}}u^\dagger(\mathbf{p},s_3)\int d^3x\,e^{-i\mathbf{px}}\psi(x),\\ b^\dagger_{\mathbf{p},s_3} &= e^{-ip^0x^0}\frac{1}{\sqrt{Vp^0/M}}v^\dagger(\mathbf{p},s_3)\int d^3x\,e^{i\mathbf{px}}\psi(x), \end{aligned} \tag{5.213}$$

this being the analog of the scalar equations (5.6), (5.73). The same result can of course be obtained from (5.210) with the help of the scalar products (3.603), in terms of which Eqs. (5.213) are simply

$$a_{\mathbf{p},s_3} = (f_{\mathbf{p}\,s_3},\psi)_t, \qquad b^\dagger_{\mathbf{p},s_3} = (f^c_{\mathbf{p}\,s_3},\psi)_t, \tag{5.214}$$

as in the scalar equations (5.19).

From (5.213) we derive that all anticommutators between $a_{\mathbf{p},s_3}$, $a^\dagger_{\mathbf{p}',s_3'}$, $b_{\mathbf{p},s_3}$, $b^\dagger_{\mathbf{p}',s_3'}$ vanish, except for

$$\left\{a_{\mathbf{p},s_3}, a^\dagger_{\mathbf{p}',s_3'}\right\} = \sqrt{\frac{M}{p^0}\frac{M}{p^{0\prime}}}u^\dagger(\mathbf{p},s_3)u(\mathbf{p}',s_3')\delta_{\mathbf{p},\mathbf{p}'} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{s_3,s_3'}, \tag{5.215}$$

$$\left\{b_{\mathbf{p},s_3}, b^\dagger_{\mathbf{p}',s_3'}\right\} = \sqrt{\frac{M}{p^0}\frac{M}{p^{0\prime}}}v^\dagger(\mathbf{p},s_3)v(\mathbf{p},s_3)\delta_{\mathbf{p},\mathbf{p}'} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{s_3,s_3'}. \tag{5.216}$$

The single-particle states

$$|\mathbf{p},s_3\rangle = a^\dagger_{\mathbf{p},s_3}|0\rangle \tag{5.217}$$

have the wave functions

$$\begin{aligned} \langle 0|\psi(x)|\mathbf{p},s_3\rangle &= \frac{1}{\sqrt{Vp^0/M}}e^{-ipx}u(\mathbf{p},s_3) = \mathrm{f}_{\mathbf{p},s_3}(x)\\ \langle \mathbf{p},s_3|\bar\psi(x)|0\rangle &= \frac{1}{\sqrt{Vp^0/M}}e^{ipx}\bar u(\mathbf{p},s_3) = \bar{\mathrm{f}}_{\mathbf{p},s_3}(x). \end{aligned} \tag{5.218}$$

In addition, there are states

$$|\bar{\mathbf{p}},s_3\rangle = b^\dagger_{\mathbf{p},s_3}|0\rangle, \tag{5.219}$$

with the matrix elements

$$\begin{aligned} \langle \bar{\mathbf{p}}s_3|\psi(x)|0\rangle &= \frac{1}{\sqrt{Vp^0/M}}e^{ipx}v(\mathbf{p},s_3) = \mathrm{f}^c_{\mathbf{p},s_3}(x),\\ \langle 0|\bar\psi(x)|\bar{\mathbf{p}},s_3\rangle &= \frac{1}{\sqrt{Vp^0/M}}e^{-ipx}\bar u(\mathbf{p},s_3) = \bar{\mathrm{f}}^c_{\mathbf{p},s_3}(x). \end{aligned} \tag{5.220}$$

As in the scalar field expansion (5.72), the association of the negative-frequncy solution $v(\mathbf{p},s_3)e^{ipx}$ of the Dirac equation with a creation operator $b^\dagger_{\mathbf{p},s_3}$ rather than a second annihilation operator $d_{-\mathbf{p},-s_3}$ ensures that the wave equation of the particle $|\bar{\mathbf{p}}s_3\rangle$ has the same exponential form e^{-ipx} as that of $|\mathbf{p},s_3\rangle$, both exhibiting the same time dependence e^{-p^0t} with the positive energy $p^0=\omega_{\mathbf{p}}$. The other assignment would have given a negative energy.

In an infinite volume, a more convenient field expansion makes use of the plane-wave solutions (3.605) and uses covariant creation and annihilation operators as in (5.16):

$$\psi(x)=\int\frac{d^3p}{(2\pi)^3p^0/M}\sum_{s_3}\left[e^{-ipx}u(\mathbf{p},s_3)\mathrm{a}_{\mathbf{p},s_3}+e^{ipx}v(\mathbf{p},s_3)\mathrm{b}^\dagger_{\mathbf{p},s_3}\right]. \tag{5.221}$$

The commutation rules between $\mathrm{a}_{\mathbf{p},s_3}$, $\mathrm{a}^\dagger_{\mathbf{p},s_3}$, $\mathrm{b}_{\mathbf{p},s_3}$, and $\mathrm{b}^\dagger_{\mathbf{p},s_3}$ are the same as in (5.215), (5.216), but with the replacement of the Kronecker symbols by their invariant continuum version [recall (5.20)]

$$\delta_{\mathbf{p},\mathbf{p}'}\rightarrow\frac{p^0}{M}\,\delta^{(3)}(\mathbf{p}-\mathbf{p}')=\frac{p^0}{M}(2\pi\hbar)^D\,\delta^{(3)}(\mathbf{p}-\mathbf{p}'). \tag{5.222}$$

Note that this normalization is different from the bosonic one in (5.20), where the factor in front of the δ-function was $2p^0$. This is a standard convention spread throughout the literature.

As for scalar fields, we introduce single-particle states

$$|\mathbf{p},s_3)=\mathrm{a}^\dagger_{\mathbf{p},s_3}|0),\qquad|\bar{\mathbf{p}},s_3)=\mathrm{b}^\dagger_{\mathbf{p},s_3}|0), \tag{5.223}$$

with the vacuum $|0)$ defined by $\mathrm{a}_{\mathbf{p},s_3}|0)=0$ and $\mathrm{b}_{\mathbf{p},s_3}|0)=0$. These states will be satisfy the orthogonality relations

$$(\mathbf{p}',s_3'|\mathbf{p},s_3)=\frac{p^0}{M}\,\delta^{(3)}(\mathbf{p}'-\mathbf{p})\delta_{s_3',s_3},\qquad(\bar{\mathbf{p}}',s_3'|\bar{\mathbf{p}},s_3)=\frac{p^0}{M}\,\delta^{(3)}(\mathbf{p}'-\mathbf{p})\delta_{s_3',s_3}, \tag{5.224}$$

in accordance with the replacement (5.222), and in contrast to (5.26). They have the wave functions

$$\begin{array}{ll}(0|\psi(x)|\mathbf{p},s_3)=e^{-ipx}u(\mathbf{p},s_3)=\mathrm{f}_{\mathbf{p},s_3}(x), & (\mathbf{p},s_3|\bar{\psi}(x)|0)=e^{ipx}\bar{u}(\mathbf{p},s_3)\;=\bar{\mathrm{f}}_{\mathbf{p},s_3}(x).\\ (\bar{\mathbf{p}},s_3|\psi(x)|0)=e^{ipx}v(\mathbf{p},s_3)\;=\mathrm{f}^c_{\mathbf{p},s_3}(x), & \langle 0|\bar{\psi}(x)|\bar{\mathbf{p}},s_3\rangle=e^{-ipx}\bar{v}(\mathbf{p},s_3)=\bar{\mathrm{f}}^c_{\mathbf{p},s_3}(x).\end{array} \tag{5.225}$$

We end this section by stating also the explicit form of the quantized field of massless left-handed neutrinos and their antiparticles, the right-handed antineutrinos:

$$\psi^\nu(x)=\frac{1-\gamma_5}{2}\psi(x)=\sum_{\mathbf{p}}\frac{1}{\sqrt{2Vp^0}}\left[e^{-ipx}u_L(\mathbf{p})a_{\mathbf{p},-\frac{1}{2}}+e^{ipx}v_R(\mathbf{p})b^\dagger_{\mathbf{p},\frac{1}{2}}\right], \tag{5.226}$$

where the operators $a^\dagger_{\mathbf{p},-\frac{1}{2}}$ and $b^\dagger_{\mathbf{p},\frac{1}{2}}$ carry helicity labels $\mp\frac{1}{2}$, and $p^0=|\mathbf{p}|$. The massless helicity bispinors are those of Eqs. (3.665) and (3.666). Remember the normalization (3.664):

$$\begin{array}{ll} u_L^\dagger(\mathbf{p})u_L(\mathbf{p})=2p^0, & u_R^\dagger(\mathbf{p})u_R(\mathbf{p})=2p^0, \\ v_L^\dagger(\mathbf{p})v_L(\mathbf{p})\ =2p^0, & v_R^\dagger(\mathbf{p})v_R(\mathbf{p})\ =2p^0, \end{array} \tag{5.227}$$

which is the reason for the factor $1/\sqrt{2Vp^0}$ in the expansion (5.226) [as in the expansions (5.12) and (5.72) for the scalar mesons].

5.3.2 Energy of Free Dirac Particles

We now turn to the energy of the free quantized Dirac field. The energy density is given by the Legendre transform of the Lagrangian density

$$\begin{aligned} \mathcal{H}(x) &= \pi(x)\dot{\psi}(x)-\mathcal{L}(x) \\ &= i\psi^\dagger(x)\dot{\psi}(x)-\mathcal{L}(x) \\ &= \bar{\psi}(x)i\gamma^i\partial^i\psi(x)+M\bar{\psi}(x)\psi(x). \end{aligned} \tag{5.228}$$

Inserting the expansion (5.211) and performing the spatial integral [recall the step from (5.29) to (5.30)], the double sum over momenta reduces to a single sum, and we obtain the second-quantized Hamilton operator

$$\begin{aligned} H=\sum_{\mathbf{p},s_3,s_3'}\frac{M}{p^0}\Big[& a^\dagger{}_{\mathbf{p},s_3}a_{\mathbf{p},s_3'}\bar{u}(\mathbf{p},s_3)(\gamma^ip^i+M)u(\mathbf{p},s_3') \\ & +b_{\mathbf{p},s_3}b^\dagger_{\mathbf{p},s_3'}\bar{v}(\mathbf{p},s_3)(-\gamma^ip^i+M)v(\mathbf{p},s_3') \\ & +a^\dagger{}_{\mathbf{p},s_3}b^\dagger_{-\mathbf{p},s_3'}\bar{u}(\mathbf{p},s_3)(\gamma^ip^i+M)v(-\mathbf{p},s_3')e^{2ip^0t} \\ & +b_{-\mathbf{p},s_3}a_{\mathbf{p},s_3'}\bar{v}(-\mathbf{p},s_3)(\gamma^ip^i+M)u(\mathbf{p},s_3')e^{2ip^0t}\Big]. \end{aligned} \tag{5.229}$$

We now use the Dirac equation, according to which

$$\begin{aligned} (\gamma^ip^i+M)u(\mathbf{p},s_3) &= \gamma^0p^0u(\mathbf{p},s_3), \\ (-\gamma^ip^i+M)v(\mathbf{p},s_3) &= -\gamma^0p^0v(\mathbf{p},s_3), \end{aligned} \tag{5.230}$$

and the orthogonality relations (3.635)–(3.638) and simplify (5.230) to

$$H=\sum_{\mathbf{p},s_3}p^0\left(a^\dagger_{\mathbf{p},s_3}a_{\mathbf{p},s_3}-b_{\mathbf{p},s_3}b^\dagger_{\mathbf{p},s_3}\right). \tag{5.231}$$

With the help of the anticommutation rule (5.216), this may be rewritten as

$$H=\sum_{\mathbf{p},s_3}p^0\left(a^\dagger_{\mathbf{p},s_3}a_{\mathbf{p},s_3}+b^\dagger_{\mathbf{p},s_3}b_{\mathbf{p},s_3}\right)-\sum_{\mathbf{p},s_3}p^0. \tag{5.232}$$

The total energy adds up all single-particle energies. In contrast to the second-quantized scalar field, the vacuum has now a negatively infinite energy due to the zero-point oscillations, as announced in the discussion of Eq. (5.35).

Note that if we had used here the annihilation operators of negative energy states $d_{-\mathbf{p},-s_3}$ instead of the creation operators $b^\dagger_{\mathbf{p},s_3}$, then the energy would have read

$$H = \sum_{\mathbf{p},s_3} p^0 \left(a^\dagger_{\mathbf{p},s_3} a_{\mathbf{p},s_3} - d^\dagger_{\mathbf{p},s_3} d_{\mathbf{p},s_3} \right) \tag{5.233}$$

so that the particles created by $d^\dagger_{\mathbf{p},s_3}$ would again have had negative energies. By going over from $d_{-\mathbf{p},-s_3}$ to $b^\dagger_{\mathbf{p},s_3}$, we have transformed missing negative energy states into states of antiparticles, thereby obtaining a positive sign for the energy of an antiparticle. This happens, however, at the expense of having an negatively infinite zero-point energy of the vacuum. This also explains why the spin orientation s_3 changes sign under the above replacement. A missing particle with spin down behaves like a particle with spin up.

Actually, the above statements about the exchange $d_{\mathbf{p},s_3} \to b^\dagger_{\mathbf{p},s_3}$ are correct only as far as the sum of all momentum states and spin indices s_3 in (5.233) is concerned. For a single state, we have to consider also the momentum operator and the spin.

The situation is the same as in the free-electron approximation to the electrons in a metal. At zero temperature, the electrons are in the ground state, forming a Fermi sea in which all single-particle levels below a Fermi energy E_F are occupied. If the energies are measured from that energy, all occupied levels have a negative energy, and the ground state has a large negative value. If an electron is kicked out from one of the negative-energy states, an electron-hole pair is observed, both particle and hole carrying a positive energy with respect to the undisturbed Fermi liquid. The hole appears with a positive charge relative to the Fermi sea.

Note also that unlike the Bose case, the exchange $d_{-\mathbf{p},-s_3} \to b^\dagger_{\mathbf{p},s_3}$ maintains the correct sign of canonical anticommutation rules (5.216). In fact, the negative sign of the term $-d^\dagger_{\mathbf{p},s_3} d_{\mathbf{p},s_3}$ in the Hamilton operator (5.233) is somewhat less devastating than in the Bose case. It can actually be avoided by a mere redefinition of the vacuum as the state in which all momenta are occupied by a $d^\dagger_{\mathbf{p},s_3}$ particle:

$$|0\rangle_{\text{new}} = \prod_{\mathbf{p},s_3} d^\dagger_{\mathbf{p},s_3} |0\rangle. \tag{5.234}$$

This state has now the same negatively infinite energy

$$E_{0\ \text{new}} \equiv {}_{\text{new}}\langle 0|H|0\rangle_{\text{new}} = -\sum_{\mathbf{p},s_3} p^0 \tag{5.235}$$

which was found in the correct quantization. Counting from this ground state energy, all other states have positive energies, obtained either by adding a particle with the operator $a^\dagger_{\mathbf{p},s_3}$ or by removing a particle with $d_{-\mathbf{p},-s_3}$. Of course, this description is just a reflection of the fact that for anticommutators, $-d^\dagger_{\mathbf{p},s_3} d_{\mathbf{p},s_3} = d_{\mathbf{p},s_3} d^\dagger_{\mathbf{p},s_3} - 1$, and a reinterpretation $d_{-\mathbf{p},-s_3} \to b^\dagger_{\mathbf{p},s_3}$ and $d^\dagger_{-\mathbf{p},-s_3} \to b_{\mathbf{p},s_3}$ makes $d_{\mathbf{p},s_3} d^\dagger_{\mathbf{p},s_3}$ a positive operator. For commutators, the same trick is impossible since $-d^\dagger_{\mathbf{p},s_3}d_{\mathbf{p},s_3}$ can have *any* negative eigenvalue and no new "zero level" can be given so that all energy differences are positive!

It was the major discovery of Dirac that the annihilation of a negative-energy particle may be viewed as a creation of a positive-energy particle with the same mass and spin, but reversed directions of momentum and spin. Dirac called it the *antiparticle*. When dealing with electrons, the antiparticle is a *positron*. Dirac imagined all negative energy states in the world as being filled, forming a sea of negative energy states, just in the above-described Fermi sea in metals. as the electrons below the Fermi surface in a metal. The annihilation of a negative-energy particle in the sea would create a hole which would appear to the observer as a particle of positive energy with the opposite charge.

As in the scalar case it is often possible to simply drop this infinite energy of the vacuum by introducing a normal product $:\mathcal{H}:$. As before, the double dots mean: Order all operators such that all creators stand to the left of all annihilators. But in contrast to the boson case, every transmutation of two Fermi operators to achieve the normal order is now accompanied by a phase factor -1.

5.3.3 Lorentz Transformation Properties of Particle States

The behavior of the bispinors $u(\mathbf{p},s_3)$ and $v(\mathbf{p},s_3)$ under Lorentz transformations determines the bahavior of the creation and annihilation operators of particles and antiparticles, and thus of the particle states created by them, in particular the single-particle states (5.217) and (5.219). Under a Lorentz transformation Λ, the field operator $\psi(x)$ transforms according to the law (3.475):

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = D(\Lambda)\psi(\Lambda^{-1}x) = e^{-i\frac{1}{2}\omega_{\mu\nu}S^{\mu\nu}}\psi(\Lambda^{-1}x), \tag{5.236}$$

On the right-hand side, we now insert the expansion (5.221), it becomes

$$\begin{aligned} D(\Lambda)\psi(\Lambda^{-1}x) = \int \frac{d^3p}{(2\pi)^3p^0/M} \sum_{s_3,s_3'} \Big[& e^{-ip'x}u(\mathbf{p}',s_3')W_{s_3',s_3}(p',\Lambda,p)\,\mathrm{a}_{\mathbf{p},s_3} \\ & + e^{ip'x}v(\mathbf{p}',s_3')W^*_{s_3',s_3}(p',\Lambda,p)\,\mathrm{b}^\dagger_{\mathbf{p},s_3}\Big]. \end{aligned}$$

where we have set $p' \equiv \Lambda p$ and used the fact that $p\Lambda^{-1}x = p'x$. In order to derive the transformation laws for the creation and annihilation operators, we rewrite this in the same form as in the original expansion (5.221) in primed quantities.

$$D(\Lambda)\psi(\Lambda^{-1}x) = \int \frac{d^3p'}{(2\pi)^3p'^0/M} \sum_{s_3,s_3'} \left[e^{-ip'x}u(\mathbf{p}',s_3')\mathrm{a}'_{\mathbf{p}',s_3'} + e^{ip'x}v(\mathbf{p}',s_3')\mathrm{b}'^\dagger_{\mathbf{p}',s_3'}\right], \tag{5.237}$$

Because of the Lorentz invariance of the integration measure in momentum space observed in (3.176), we can replace in (5.237)

$$\int \frac{d^3p}{(2\pi)^3p^0/M} \to \int \frac{d^3p}{(2\pi)^3p'^0/M}, \tag{5.238}$$

and compare coefficients to find the transformation laws

$$\begin{aligned}
\mathrm{a}_{\mathbf{p}',s_3'} \quad &\xrightarrow{\Lambda} \quad \mathrm{a}'_{\mathbf{p}',s_3'} = \sum_{s_3=-1/2}^{1/2} W_{s_3',s_3}(p',\Lambda,p)\,\mathrm{a}_{\mathbf{p},s_3},\\
b^\dagger_{\mathbf{p}',s_3'} \quad &\xrightarrow{\Lambda} \quad \mathrm{b}'^\dagger_{\mathbf{p}',s_3'} = \sum_{s_3=-1/2}^{1/2} W^*_{s_3',s_3}(p',\Lambda,p)\,\mathrm{b}^\dagger_{\mathbf{p},s_3}.
\end{aligned} \tag{5.239}$$

In contrast to the Lorentz transformations (5.236) of the field, the creation and annihilation operators are transformed *unitarily* under the Lorentz group. The right-hand sides define a unitary representation of the Lorentz tranformations Λ:

$$\begin{aligned}
\mathrm{a}'_{\mathbf{p}',s_3'} &= \mathcal{U}^{-1}(\Lambda)\mathrm{a}_{\mathbf{p}',s_3'}\mathcal{U}(\Lambda) = \sum_{s_3=-1/2}^{1/2} W_{s_3',s_3}(p',\Lambda,p)\,\mathrm{a}_{\mathbf{p},s_3},\\
\mathrm{b}'^\dagger_{\mathbf{p}',s_3'} &= \mathcal{U}^{-1}(\Lambda)\mathrm{b}^\dagger_{\mathbf{p}',s_3'}\mathcal{U}(\Lambda) = \sum_{s_3=-1/2}^{1/2} W^*_{s_3',s_3}(p',\Lambda,p)\,\mathrm{b}^\dagger_{\mathbf{p},s_3},
\end{aligned} \tag{5.240}$$

with similar relations for $\mathrm{a}^\dagger_{\mathbf{p},s_3}$ and $\mathrm{b}_{\mathbf{p},s_3}$. For the single-particle states (5.223), this implies the transformation laws:

$$\begin{aligned}
\mathcal{U}(\Lambda)|\mathbf{p},s_3\rangle &= \mathcal{U}(\Lambda)\mathrm{a}^\dagger_{\mathbf{p},s_3}\mathcal{U}^{-1}(\Lambda)|0\rangle = \sum_{s_3'=-1/2}^{1/2} |\mathbf{p}',s_3'\rangle W_{s_3',s_3}(p',\Lambda,p),\\
\mathcal{U}(\Lambda)|\bar{\mathbf{p}},s_3\rangle &= \mathcal{U}(\Lambda)\mathrm{b}^\dagger_{\mathbf{p},s_3}\mathcal{U}^{-1}(\Lambda)|0\rangle = \sum_{s_3'=-1/2}^{1/2} |\bar{\mathbf{p}}',s_3'\rangle W_{s_3',s_3}(p',\Lambda,p),
\end{aligned} \tag{5.241}$$

where we have used the Lorentz-invariance of the vacuum state

$$\mathcal{U}(\Lambda)|0\rangle = |0\rangle. \tag{5.242}$$

We are now ready to understand the reason for introducing the matrix c in the bispinors $v(\mathbf{p},s_3)$ of Eq. (3.623), and thus of the sign reversal of the spin orientation. In (3.681) we found that the canonical spin indices of $v(\mathbf{p},s_3)$ transformed under rotations by the complex-conjugate 2×2 Wigner matrices with respect to those of $u(\mathbf{p},s_3)$. This implies that the Wigner rotations mixing the spin components of the operators $\mathrm{a}_{\mathbf{p},s_3}$ and $\mathrm{b}^\dagger_{\mathbf{p},s_3}$ are complex conjugate to each other. As a consequence, $\mathrm{b}^\dagger_{\mathbf{p},s_3}$ tranforms in the same way as $\mathrm{a}^\dagger_{\mathbf{p},s_3}$, and antiparticles behave in precisely the same way under Lorentz tansformations as particles.

For massless particles in the helicity representation, the creation and annihilation operators transform under Lorentz transformations merely by a phase factor, as discussed at the end of Section 3.16.1.

Under translations by a four-vector a^μ, the particle and antiparticle states $|\mathbf{p},s_3) = \mathrm{a}^\dagger_{\mathbf{p},s_3}|0)$ and $|\bar{\mathbf{p}},s_3) = \mathrm{b}^\dagger_{\mathbf{p},s_3}|0)$ transform rather trivially. Since they have a definite momentum, the receive merely a phase factor e^{ipa}. This follows directly by implementing the transformation law (3.478) on the Dirac field operator:

$$\psi(x) \longrightarrow \psi'(x) = \psi(x-a). \tag{5.243}$$

Inserting into the right-hand side the operator expansion (5.221), we see that the creation and annihilation operators transform as follows:

$$\begin{array}{lcl} \mathrm{a}_{\mathbf{p},s_3} & \longrightarrow & \mathrm{a}'_{\mathbf{p},s_3} = e^{ipa} \; \mathrm{a}_{\mathbf{p},s_3}, \\ \mathrm{b}^\dagger_{\mathbf{p},s_3} & \longrightarrow & \mathrm{b}'^\dagger_{\mathbf{p},s_3} = e^{-ipa}\, \mathrm{b}^\dagger_{\mathbf{p},s_3}. \end{array} \tag{5.244}$$

These transformation laws define a unitary operator of translations $\mathcal{U}(a)$:

$$\begin{array}{lcl} a'_{\mathbf{p},s_3} & = & \mathcal{U}^{-1}(a)\mathrm{a}_{\mathbf{p},s_3}\mathcal{U}(a) = e^{ipa} \; \mathrm{a}_{\mathbf{p},s_3}, \\ \mathrm{b}'^\dagger_{\mathbf{p},s_3} & = & \mathcal{U}^{-1}(a)\mathrm{b}^\dagger_{\mathbf{p},s_3}\mathcal{U}(a) = e^{-ipa}\, \mathrm{b}^\dagger_{\mathbf{p},s_3}. \end{array} \tag{5.245}$$

On the single-particle states, the operator $\mathcal{U}(a)$ has the effect:

$$\begin{array}{lcl} \mathcal{U}(a)|\mathbf{p},s_3\rangle & = & \mathcal{U}(a)\mathrm{a}^\dagger_{\mathbf{p},s_3}\mathcal{U}^{-1}(a)|0\rangle = |\mathbf{p},s_3\rangle e^{ipa}, \\ \mathcal{U}(a)|\bar{\mathbf{p}},s_3\rangle & = & \mathcal{U}(a)\mathrm{b}^\dagger_{\mathbf{p},s_3}\mathcal{U}^{-1}(\Lambda)|0\rangle = |\bar{\mathbf{p}},s_3\rangle e^{ipa}. \end{array} \tag{5.246}$$

One can immediately write down an explicit expression for this operator:

$$\mathcal{U}(a) = e^{iaP}, \tag{5.247}$$

where P^0 is the Hamilton operator (5.232), rewritten in the infinite-volume form as

$$P^0 \equiv H = \int \frac{d^3p}{(2\pi)^3 p^0/M} \left(\mathrm{a}^\dagger_{\mathbf{p},s_3} p^0 \, \mathrm{a}_{\mathbf{p},s_3} + \mathrm{b}^\dagger_{\mathbf{p},s_3} p^0 \, \mathrm{b}_{\mathbf{p},s_3} - p^0 \frac{p^0}{M} \, \delta^{(3)}(\mathbf{0}) \right). \tag{5.248}$$

The last term is a formal infinite-volume expression for the finite-vlolume vacuum energy

$$P^0_{\text{vac}} = -\int \frac{d^3pV}{(2\pi)^3} p^0, \tag{5.249}$$

as we see from the Fourier respresentation of $\delta^{(3)}(\mathbf{p}) = \int d^3x \, e^{i\mathbf{p}\mathbf{x}}$ which is equal to V for $\mathbf{p} = 0$. The operator of total momentum reads

$$\mathbf{P} \equiv \int \frac{d^3p}{(2\pi)^3 p^0/M} \left(\mathrm{a}^\dagger_{\mathbf{p},s_3} \, \mathbf{p} \, \mathrm{a}_{\mathbf{p},s_3} + \mathrm{b}^\dagger_{\mathbf{p},s_3} \, \mathbf{p} \, \mathrm{b}_{\mathbf{p},s_3} \right). \tag{5.250}$$

Together, they form the operator of total four-momentum $P^\mu = (P^0, \mathbf{P})$ which satisfies the commutation rules with the particle creation and annihilation operators

$$[P^\mu, \mathrm{a}^\dagger_{\mathbf{p},s_3}] = p^\mu \, \mathrm{a}^\dagger_{\mathbf{p},s_3}, \qquad [P^\mu, \mathrm{b}^\dagger_{\mathbf{p},s_3}] = p^\mu \, \mathrm{b}^\dagger_{\mathbf{p},s_3}. \tag{5.251}$$

These express the fact that by adding a particle of energy and momentum p^μ to the system, the total energy and momentum P^μ is increased by p^μ.

By combining Lorentz transformations and translations as in (3.480), we cover the entire Poincaré group, and the single-particle states form an irreducible representation space of this group. The invariants of the representation are the mass $M = \sqrt{p^2}$ and the spin s. Thus the complete specification of a representation state is

$$|\mathbf{p}, s_3[M, s]\rangle. \tag{5.252}$$

The Hilbert space of two-particle states $|\mathbf{p}, s_3[M, s]; \mathbf{p}', s_3'[M', s']\rangle$ gives rise to a reducible representation of the Poincaré group. The reducibility is obvious from the fact that if both particles are at rest, the state $|\mathbf{0}, s_3[M, s]; \mathbf{0}', s_3'[M', s']\rangle$ is simply a product of two rotational states of spins s and s', and decomposes into irreducible representations of the rotation group with spins $S = |s - s'|, |s - s'| + 1, \ldots, s + s'$. If the two particles carry momenta, the combined state will also have all possible orbital angular momenta. In the center-of-mass frame of the two particles, the momenta are of equal size and point in opposite directions. The states are then characterized by the direction of one of the momenta, say $\hat{\mathbf{p}}$, and may be written as $|\hat{\mathbf{p}}, s_3, s_3'\}$. The satisfy the completeness relation

$$\sum_{s_3=-s}^{s} \sum_{s_3'=-s'}^{s'} \int_0^\pi d\theta \int_0^{2\pi} d\varphi \; |\hat{\mathbf{p}}, s_3, s_3'\}\{\hat{\mathbf{p}}, s_3, s_3'| = 1, \tag{5.253}$$

where θ and φ are the spherical angles of the direction $\hat{\mathbf{p}}$.

In the absence of spin, it is then simple to find the irreducible contents of the rotation group. We merely expand the state $|\hat{\mathbf{p}}\}$ in partial waves:

$$|\hat{\mathbf{p}}\} = \sum_{l,m} |l, m\}\{l, m|\hat{\mathbf{p}}\} \equiv \sum_{l,m} |l, m\} Y_{lm}(\theta, \phi), \tag{5.254}$$

with spherical harmonics $Y_{l,m}(\theta, \phi)$. The states $|j, m\}$ are orthonormal and complete in this Hilbert space:

$$\{j, m|j', m'\} = \delta_{j,j'}\delta_{m,m'}, \qquad \sum_{j,m} |j, m\}\{j, m| = 1. \tag{5.255}$$

In the presence of spins s, s', the decomposition is simplest if the spin orientations are specified in the helicity basis. Then the two-particle states possess an azimuthal angular momentum of size $h - h'$ around the direction $\hat{\mathbf{p}}$, and may be written as $|\hat{\mathbf{p}}, h - h'\}$. These have the same rotation properties the wave functions of a spinning top with an azimuthal angular momentum $h - h'$ around the body axis. The latter functions are well known — they are just the representation functions

$$D^j_{m\,m'}(\alpha, \beta, \gamma) = e^{-i(m\alpha + m'\gamma)} d^j_{m\,m'}(\beta) \tag{5.256}$$

of rotations of angular momentum j introduced in Eq. (3.800). These serve as wave functions of a spinning top with angular momentum j and magnetic quantum number m, and with an azimuthal component m' of angular momentum around the body axis. They are the basis states of irreducible representations of the rotation group in the center-of-mass frame. Thus, extending (5.254), we can expand

$$\begin{aligned} |\hat{\mathbf{p}}, h-h'\} &= \sum_{j,m} |j,m,h-h'\}\{j,m,h-h'|\hat{\mathbf{p}}\} \\ &\equiv \sum_{j,m} |j,m,h-h'\}\sqrt{\frac{2j+1}{4\pi}}D^{j}_{m\,h-h'}(\varphi,\theta,0), \end{aligned} \tag{5.257}$$

with an orthonormal and complete set of states $|j,m,h-h'\}$ at a fixed $h-h'$. The normalization factor is determined to comply with the orthonormality property (3.820) of the rotation functions.

Now we boost this expansion from the center-of-mass frame back to the initial frame in which the total momentum is $\mathbf{P}=\mathbf{p}+\mathbf{p}'$, the energy $P^0=p^0+p'^0$, and the mass $\mu=\sqrt{P^2}$. The direction of $\mathbf{P}$ may be chosen as a quantization axis for the angular momentum j. Then the quantum number m is equal to the helicity of the combined state. The angular momentum j in the rest frame determines the spin of the combined state. The resulting Clebsch-Gordan-like expansion of the two-particle state into irreducible representations of the Poincaré group is

$$\begin{aligned} |\mathbf{p}, s_3\,[M,s]\,;\mathbf{p}', s_3'\,[M,s']\,\rangle &= \sum_{j,m}\int\limits_{(M+M')^2}^{\infty}\frac{d\mu}{2\pi}\int\frac{d^3P}{(2\pi)^3P^0/\mu}\,|\mathbf{P},m\,[\mu,j]\,\eta\rangle \\ &\quad\times\langle\mathbf{P},m\,[\mu,j]\,\eta|\mathbf{p},s_3\,[M,s]\,;\mathbf{p}',s_3'\,[M',s']\,\rangle, \end{aligned} \tag{5.258}$$

with the expansion coefficients

$$\begin{aligned} \langle\mathbf{P},m\,[\mu,j]\,\eta|\mathbf{p},h\,[M,s]\,;\mathbf{p}',h'\,[M',s']\,\rangle &= \delta^{(4)}(P-p-p')\,\mathcal{N}(\mu;M,M') \\ &\quad\times\frac{2j+1}{4\pi}D^{j}_{m\,h-h'}(\varphi,\theta,0), \end{aligned} \tag{5.259}$$

where $\mathcal{N}(\mu;M,M')$ is some normalization factor. The product representation is not simply reducible and requires distinguishing the different irreducible *biparticle states* of spin S. For this purpose, a degeneracy label η has been introduced. It may be taken as the pair of helicity indices $(h.h')$ of the individual particles which the biparticle is composed of. However, to describe different processes most efficiently, other linear combinations may be more convenient. One may, for example, combine first the individual spins to a total intermediate spin S, then this with the orbital angular momentum L in the center-of-mass frame to the final total angular momentum that frame j (the spin of the biparticle). This corresponds to the LS coupling scheme in atomic physics. Explicitly, these states are

$$|\mathbf{P},m\,[\mu,j]\,(LS)\rangle=\langle j,h{-}h'|L,0;S,h{-}h'\rangle\langle S,h{-}h'|s,h;s',-h'\rangle|\mathbf{P},m\,[\mu,j]\,(h,h')\rangle. \tag{5.260}$$

A sum over all h,h' is implied. Since the quantization axis is the direction of $\mathbf{p}$ in the center-of-mass frame, the orbital angular momentum has no L_3-component.

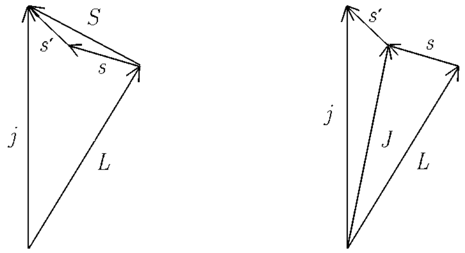

FIGURE 5.4 Different coupling schemes for two-particle states of total angular momentum j and helicity m. The first is the LS, the second the JL scheme.

Another possibility of coupling the two particles corresponds to the multipole radiation in electromagnetism. Here one of the particles, say $[M,s]$, is singled out to carry off radiation, which is analyzed according to its total angular momentum J composed of L and s. This total angular momentum is coupled with the other spin s' to the combined total angular momentum j of the biparticle. Here the states are

$$|\mathbf{P},m\,[\mu,j]\,(JL)\rangle = \langle J,h|s,h;L,0\rangle\langle j,h-h'|J,h;s',-h'\rangle|\mathbf{P},m\,[\mu,j]\,(h,h')\rangle. \quad (5.261)$$

As in (5.260), a sum over all h,h' is implied. The (LS) and (JL) states are related to each other by *Racah's recoupling coefficients.*[15].

The integral over μ can be performed after decomposing the δ-function ensuring the conservation of energy and momentum as

$$\delta^{(4)}(P-p-p') = \delta^{(3)}(\mathbf{P}-\mathbf{p}-\mathbf{p}')\,\delta\left(\mu-\sqrt{(p+p')^2}\right)\frac{P^0}{\mu}. \quad (5.262)$$

A suitable normalization of the irrducible states is

$$\langle\mathbf{P},m\,[\mu,j]\,\eta|\mathbf{P}',m'\,[\mu',j']\,\eta'\rangle = \delta^{(3)}(\mathbf{P}-\mathbf{P}')\,\delta(\mu-\mu')\delta_{j,j'}\delta_{m,m'}\delta_{\eta,\eta'}. \quad (5.263)$$

For more details on this subject see Notes and References.

Propagator of Free Dirac Particles

Let us now use the quantized field to calculate the propagator of the free Dirac field. Thus we form the vacuum expectation value of the time ordered product

$$S(x,x') = \langle 0|T\psi(x)\bar\psi(x')|0\rangle. \quad (5.264)$$

For, if we use the explicit decomposition

$$T\psi(x)\bar\psi(x') \;=\; \Theta(x_0-x_0')\psi(x)\bar\psi(x') - \Theta(x_0'-x_0)\bar\psi(x')\psi(x) \quad (5.265)$$

---

[15] For the general recoupling theory of angular momenta see Chapter VI of the textbook by Edmonds, quoted in Notes and References of our Chapter 3

and apply the Dirac equation (3.600) we see that

$$
\begin{aligned}
&(i\gamma^\mu\partial_\mu - M)T\psi(x)\bar\psi(x')\\
&\quad = T(i\gamma^\mu\partial_\mu - M)\psi(x)\psi(x') + i\delta(x_0 - x_0')\left\{\gamma_0\psi(x), \bar\psi(x')\right\}. \qquad (5.266)
\end{aligned}
$$

The right-hand side reduces indeed to $i\delta^{(4)}(x-x')$, due to the Dirac equation (5.204) and the canonical commutation relation (5.209).

Let us now insert the free-field expansion (5.211) into (5.264) and calculate, in analogy to (5.44),

$$
\begin{aligned}
&S_{\alpha\beta}(x,x') = S_{\alpha\beta}(x-x')\\
&\quad = \Theta(x_0 - x_0')\frac{1}{V}\sum_{\mathbf{p},s_3;\mathbf{p}',s_3}\frac{M}{\sqrt{p^0p^{0\prime}}}e^{i(px-p'x')}u_\alpha(\mathbf{p},s_3')\bar u_\beta(\mathbf{p}',s_3')\langle 0|a_{\mathbf{p},s_3}a^\dagger_{\mathbf{p}',s_3'}|0\rangle\\
&\qquad -\Theta(x_0' - x_0)\frac{1}{V}\sum_{\mathbf{p},s_3;\mathbf{p}',s_3}\frac{M}{\sqrt{p^0p^{0\prime}}}e^{i(px-p'x')}v_\alpha(\mathbf{p},s_3)\bar v_\beta(\mathbf{p}',s_3')\langle 0|b_{\mathbf{p}',s_3'}b^\dagger_{\mathbf{p},s_3'}|0\rangle\\
&\quad = \Theta(x_0 - x_0')\frac{1}{V}\sum_{\mathbf{p},s_3}\frac{M}{p^0}e^{-ip(x-x')}\sum_{s_3}u_\alpha(\mathbf{p},s_3)\bar u_\beta(\mathbf{p},s_3)\\
&\qquad -\Theta(x_0' - x_0)\frac{1}{V}\sum_{\mathbf{p},s_3}\frac{M}{p^0}e^{ip(x-x')}\sum_{s_3}v_\alpha(\mathbf{p},s_3)\bar v_\beta(\mathbf{p},s_3) \qquad (5.267)
\end{aligned}
$$

We now recall the polarization sums (3.641) and (3.642), and obtain from (5.267),

$$
\begin{aligned}
S_{\alpha\beta}(x-x') &= \Theta(x_0 - x_0')\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{-ip(x-x')}(\not p + M)\\
&+ \Theta(x_0' - x_0)\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{ip(x-x')}(-\not p + M). \qquad (5.268)
\end{aligned}
$$

Let us mention here that this type of decomposition can be found for particles of any spin. In (3.644) we introduced the polarization sum

$$
P(p) = \sum_{s_3}u(\mathbf{p},s_3)\bar u(\mathbf{p},s_3), \qquad \bar P(p) = \sum_{s_3}v(\mathbf{p},s_3)\bar v(\mathbf{p},s_3) = -P(-p). \qquad (5.269)
$$

In terms of these, the propagator has the general form

$$
\begin{aligned}
S_{\alpha\beta}(x-x') &= \Theta(x_0 - x_0')\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{-ip(x-x')}P(p)\\
&+ \Theta(x_0' - x_0)\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{ip(x-x')}P(-p). \qquad (5.270)
\end{aligned}
$$

This structure is found for particles of any spin, in particular also for integer-valued ones. The alternating sign in relation (3.645) between the polarization sums of particles and antiparticles is cancelled by the alternating sign in the definition of the time-ordered product for bosons and fermions, if the statistics is chosen properly. This will be discussed in more detail in Section 5.8.

In an infinite volume, the momentum sums are replaced by integrals and yield the invariant functions $G^{(+)}(x-x'), G^{(-)}(x-x')$ [recall (5.45) and (5.52)]. The sum containing the term $\not p$ may be summed in this way after taking it outside in form of a spacetime derivative, i.e., by writing

$$\frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{p^0}e^{\mp ip(x-x')}(\pm\not p + M) = (\pm i\not\partial + M)G^{(\pm)}(x-x'). \tag{5.271}$$

Note that the zeroth component inside the sum comes from the polarization sum over spinors and thus lies *on the mass shell*, and that also the Green functions $G^{(+)}(x-x')$ and $G^{(-)}(x-x')$ contain only wave functions with on-shell energies. We therefore find the propagator

$$S_{\alpha\beta}(x-x') = \Theta(x_0-x_0')(i\not\partial + M)G^{(+)}(x-x') + \Theta(x_0'-x_0)(i\not\partial + M)G^{(-)}(x-x'). \tag{5.272}$$

This expression can be simplified further by moving the derivatives to the left of the Heaviside function. This gives

$$\begin{aligned} S_{\alpha\beta}(x-x') &= (i\not\partial + M)\left[\Theta(x_0-x_0')G^{(+)}(x-x') + \Theta(x_0'-x_0)G^{(-)}(x-x')\right] \\ & \quad -i\gamma^0\delta(x_0-x_0')\left[G^{(+)}(x-x') - G^{(-)}(x-x')\right] \end{aligned} \tag{5.273}$$

The second term happens to vanish because of the property

$$G^{(+)}(\mathbf{x},0) = G^{(-)}(\mathbf{x},0). \tag{5.274}$$

The final result is therefore the simple expression

$$S_{\alpha\beta}(x-x') = (i\not\partial + M)G(x-x'), \tag{5.275}$$

i.e., the propagator of the Dirac field reduces to that of the scalar field multiplied by the differential operator $i\not\partial + M$. Inserting on the right-hand side the Fourier representation (5.63) of the scalar propagator, we find for Dirac particles the representation

$$S_{\alpha\beta}(x-x') = \int\frac{d^4p}{(2\pi)^4}(\not p + M)\frac{i}{p^2-M^2+i\eta}e^{-ip(x-x')}. \tag{5.276}$$

This is to be contrasted with the Fourier representation of the intermediate expression (5.272). If the Heaviside functions are expressed as in Eq. (5.59), we see that (5.272) can be written as

$$S_{\alpha\beta}(x-x') = \gamma^0\int\frac{d^4p}{(2\pi)^4}\frac{i}{2\omega_{\mathbf{p}}}\left(\frac{\omega_{\mathbf{p}}}{p^0-\omega_{\mathbf{p}}+i\eta} - \frac{-\omega_{\mathbf{p}}}{p^0+\omega_{\mathbf{p}}-i\eta}\right)e^{-ip(x-x')}. \tag{5.277}$$

The difference between (5.277) and (5.276) is an integral

$$-\int \frac{dp^0}{2\pi} e^{-ip^0(x^0-x'^0)} \frac{i}{2\omega_{\mathbf{p}}} \left(\frac{p^0-\omega_{\mathbf{p}}}{p^0-\omega_{\mathbf{p}}+i\eta} - \frac{p^0+\omega_{\mathbf{p}}}{p^0+\omega_{\mathbf{p}}-i\eta} \right), \tag{5.278}$$

But the two distributions in the integrands are of the form $x/(x \pm i\eta)$, and thus equal to unity, so that (5.278) vanishes.

The integrand in (5.276) can be rewritten in a more compact way using the product formula

$$(\not{p}-M)(\not{p}+M) = p^2 - M^2. \tag{5.279}$$

This leads to the Fourier representation of the Dirac propagator

$$S_{\alpha\beta}(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{\not{p}-M+i\eta} e^{-ip(x-x')} \tag{5.280}$$

It is worth noting that while in Eq. (5.268) the particle energy k^0 in $\not{p}$ lies on the mass shell, being equal to $\sqrt{\mathbf{p}^2+M^2}$, those in the integral (5.276) lie off-shell. They are integrated over the entire k^0-axis and have no relation to the spatial momenta $\mathbf{p}$.

As in the case of the scalar fields [see Eqs. (5.352)], the free-particle propagator is equal to the Green function of the free-field equation. Indeed, by writing (3.600) as

$$L(i\partial)\psi(x) = 0 \tag{5.281}$$

with the differential operator

$$L(i\partial) = i\not{\partial} - M, \tag{5.282}$$

we see that the propagator is the Fourier transform of the inverse of $L(p)$:

$$S(x-x') = \int \frac{d^4p}{(2\pi)^4} \frac{i}{L(p)} e^{-ip(x-x')}. \tag{5.283}$$

It obviously satisfies the inhomogeneous Dirac equation

$$(i\gamma^\mu\partial_\mu - M)S(x,x') = i\delta^{(4)}(x-x'). \tag{5.284}$$

For completeness, we also write down the commutator function of Dirac fields. From the expansion (5.211) and the canonical commutation rules (5.215) and (5.216) we find directly

$$[\psi(x), \bar{\psi}(x')] \equiv C_{\alpha\beta}(x-x') \tag{5.285}$$

with the commutator function

$$\begin{aligned} C_{\alpha\beta}(x-x') &= \frac{1}{2V}\sum_{\mathbf{p}} \frac{1}{p^0} e^{-ip(x-x')}(\not{p}+M) - \frac{1}{2V}\sum_{\mathbf{p}} \frac{1}{p^0} e^{ip(x-x')}(-\not{p}+M) \\ &= (i\not{\partial}+M)C(x-x'). \end{aligned} \tag{5.286}$$

5.3.4 Behavior under Discrete Symmetries

Let us conclude this section by studying the behavior of spin $\frac{1}{2}$ particles under the discrete symmetries P, C, T.

Space Inversion

The space reflection

$$\psi(x) \xrightarrow{P} \psi'(x) = \eta_P \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \psi(\tilde{x}) = \eta_P \gamma_0 \psi(\tilde{x}) \tag{5.287}$$

is achieved by defining the unitary parity operator $\mathcal{P}$ on the creation and annihilation operators as follows:

$$\begin{aligned} \mathcal{P} a^\dagger_{\mathbf{p},s_3} \mathcal{P}^{-1} &\equiv a'^\dagger(\mathbf{p}, s_3) = \eta_P a^\dagger(-\mathbf{p}, s_3), \\ \mathcal{P} b^\dagger_{\mathbf{p},s_3} \mathcal{P}^{-1} &\equiv b'^\dagger(\mathbf{p}, s_3) = -\eta_P b^\dagger(-\mathbf{p}, s_3). \end{aligned} \tag{5.288}$$

The opposite sign in front of $b^\dagger_{\mathbf{p},s_3}$ is necessary since the spinors behave under parity as follows

$$\begin{aligned} \gamma^0 u(\mathbf{p}, s_3) &= u(-\mathbf{p}, s_3), \\ \gamma^0 v(\mathbf{p}, s_3) &= -v(-\mathbf{p}, s_3). \end{aligned} \tag{5.289}$$

This follows directly from the explicit representation (3.613) and (3.623):

$$\begin{aligned} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} \\ \sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi(s_3), \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\bar{\sigma}}{M}} \end{pmatrix} \chi^c(s_3) &= -\frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\bar{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix} \chi^c(s_3). \end{aligned} \tag{5.290}$$

It is easy to verify that with (5.288) and (5.289), the second-quantized field $\psi(x)$ with the expansion (5.211) transforms as it should:

$$\mathcal{P}\psi(x)\mathcal{P}^{-1} = \psi'_P(x) = \eta_P \gamma^0 \psi(\tilde{x}). \tag{5.291}$$

The opposite phase factors of $a^\dagger(\mathbf{p}, s_3)$ and $b^\dagger(\mathbf{p}, s_3)$ under space inversion implies that in contrast to two identical scalar particles, the bound state of a Dirac particle and its antiparticle in a relative orbital angular momentum l carries an extra minus sign, i.e., has a parity

$$\eta_P = (-)^{l+1}. \tag{5.292}$$

Therefore, the ground state of a positronium which is in an electron and a positron an s-wave bound state represents a pseudoscalar composite particle. The spins are coupled to zero.

For two different Dirac particles, the combined parity (5.292) carries, of course, an extra factor $\eta_{P_1}\eta_{P_2}$.

Charge Conjugation

Charge conjugation transforms particles into antiparticles. We therefore define this operation on the creation and annihilation operators of the Dirac particles by

$$\begin{aligned}\mathcal{C}a^\dagger_{\mathbf{p},s_3}\mathcal{C}^{-1} &= a'^\dagger_{\mathbf{p},s_3} = \eta_C b^\dagger_{\mathbf{p},s_3},\\ \mathcal{C}b^\dagger_{\mathbf{p},s_3}\mathcal{C}^{-1} &= b'^\dagger_{\mathbf{p},s_3} = \eta_C a^\dagger_{\mathbf{p},s_3}.\end{aligned} \tag{5.293}$$

To find out how this operation changes the Dirac field operator we observe that the matrix C introduces in Eq. (3.542)

$$C = i\gamma^0\gamma^2 = \begin{pmatrix} c & 0\\ 0 & -c\end{pmatrix}, \qquad c = e^{-i\pi\sigma_2/2} = -i\sigma^2, \tag{5.294}$$

has the property of changing $\bar{u}^T(\mathbf{p},s_3)$ into $v(\mathbf{p},s_3)$ and $\bar{v}^T(\mathbf{p},s_3)$ into $u(\mathbf{p},s_3)$:

$$u(\mathbf{p},s_3) = C\bar{v}^T(\mathbf{p},s_3), \qquad v(\mathbf{p},s_3) = C\bar{u}^T(\mathbf{p},s_3). \tag{5.295}$$

The second property was proved in (3.619). The fist is proved in precicely the same way.

It is then obvious that the transformation laws (5.293) have the following effect upon the second-quantized field $\psi(x)$:

$$\mathcal{C}\psi(x)\mathcal{C}^{-1} = \psi'_C(x) = \eta_C C\bar{\psi}^T(x). \tag{5.296}$$

Let us now check the transformation property of the second-quantized Dirac current $j^\mu(x)$ under charge conjugtion. In the first-quantized form we have found in Eq. (3.556) that the current ramains invariant. After field quantization, however, there is a minus sign arising from the need to interchange the order of the Dirac field operators when bringing the transformed current $\psi^T(x)\gamma^{\mu T}\bar{\psi}^T(x)$ in Eq. (3.557) back to the original operator ordering $\bar{\psi}(x)\gamma^\mu\psi(x)$ in the current $j^\mu(x)$. Thus we obtain the second-quantized tranformation law

$$j^\mu(x) \xrightarrow{C} j^{\mu\prime}(x) = -j^\mu(x). \tag{5.297}$$

rather than (3.556). This is the law listed in Table 3.1.

A bound state of a particle and its antiparticle such as the positronium in a relative angular momentum l and with the spins coupled to S has the charge parity

$$\eta_C = (-1)^{l+S}. \tag{5.298}$$

In order to see this we form the state

$$|\psi^{SS_3}_{lm}\rangle = \int_0^\infty dp\; R_l(p) \int d^2\hat{\mathbf{p}}\; Y_{lm}(\hat{\mathbf{p}}) a^\dagger_{\mathbf{p},s_3} b^\dagger_{-\mathbf{p},s'_3}|0\rangle\langle S,S_3|s,s_3;s,s'_3\rangle, \tag{5.299}$$

where $\langle S,S_3|s,s_3;s,s'_3\rangle$ are the Clebsch-Gordan coefficients coupling the two spins to a total spin S with a third component S_3 [recall Table 3.2].

Under charge conjugation, the product $a^\dagger_{\mathbf{p},s_3} b^\dagger_{-\mathbf{p},s'}$ goes over into $b^\dagger_{\mathbf{p},s_3} a^\dagger_{-\mathbf{p},s_3'}$. In order to bring this back to the original state we have to interchange the order of the two operators and the spin indices s_3 and s_3', and invert $\mathbf{p}$ into $-\mathbf{p}$. The first gives a minus sign, the second a $(-)^l$ sign, and the third a $(-)^{(S-2s_3)}$ sign, since

$$\langle S, S_3 | s, s_3; s', s_3' \rangle = (-)^{S-s-s'} \langle S, S_3 | s', s_3'; s, s_3 \rangle. \tag{5.300}$$

Altogether, this gives $(-)^{l+S}$.

Time Reversal

Under time reversal, the Dirac equation is invariant under the transformation (3.559):

$$\psi(x) \xrightarrow{T} \psi'_T(x) = D(T)\psi^*(x_T), \tag{5.301}$$

with the 4×4 -representation matrix $D(T)$ of Eq. (3.568):

$$D(T) = \eta_T C \gamma_5. \tag{5.302}$$

The second-quantized version of this tranformation of the Dirac field operators reads

$$\psi(x) \xrightarrow{T} \mathcal{T}^{-1}\psi(x)\mathcal{T} = \psi'_T(x) = D(T)\psi(-\tilde{x}), \tag{5.303}$$

The antilinearity of $\mathcal{T}$ generates the complex conjugation of the classical Dirac field in (5.301). Indeed, inserting the expansion (5.211) according to creation and annihilation operators into $\mathcal{T}^{-1}\psi(x)\mathcal{T}$, the antilinearity leads to complex-conjugate spinor wave functions:

$$\begin{aligned} \mathcal{T}^{-1}\psi(x)\mathcal{T} &= \sum_{\mathbf{p},s_3} \frac{1}{\sqrt{Vp^0/M}} \left[e^{ipx} u^*(\mathbf{p}, s_3) \mathcal{T}^{-1} a_{\mathbf{p},s_3} \mathcal{T} + e^{-ipx} v^*(\mathbf{p}, s_3) \mathcal{T}^{-1} b^\dagger_{\mathbf{p},s_3} \mathcal{T} \right] \\ &= D(T)\psi(-\tilde{x}). \end{aligned} \tag{5.304}$$

Expanding likewise the field operator $\psi(-\tilde{x})$ on the right-hand side, and comparing the Fourier coefficients, we find the equations

$$\begin{aligned} u^*(-\mathbf{p}, s_3)\mathcal{T}^{-1} a_{-\mathbf{p},s_3} \mathcal{T} &= D(T) u(\mathbf{p}, s_3) a_{\mathbf{p},s_3}, \\ v^*(-\mathbf{p}, s_3)\mathcal{T}^{-1} b^\dagger_{-\mathbf{p},s_3} \mathcal{T} &= D(T) v(\mathbf{p}, s_3) b^\dagger_{\mathbf{p},s_3}. \end{aligned} \tag{5.305}$$

To calculate the expressions on the right-hand sides we go to the chiral representations (3.613) where

$$D(T) = \eta_T C \gamma_5 = \begin{pmatrix} c & 0 \\ 0 & c \end{pmatrix}, \tag{5.306}$$

and see that

$$\begin{aligned} C\gamma_5 \, \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} c\sqrt{\frac{p\sigma}{M}} \\ c\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s_3), \\ C\gamma_5 \, \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi^c(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} c\sqrt{\frac{p\sigma}{M}} \\ -c\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi^c(s_3). \end{aligned} \tag{5.307}$$

We now proceed as in the treatment of Eq. (3.620), using relation (3.622) to find

$$\begin{aligned} C\gamma_5 \, \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ \sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ \sqrt{\frac{p\sigma}{M}} \end{pmatrix}^{*} \chi(-s_3)(-1)^{s-s_3}, \\ C\gamma_5 \, \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\sigma}{M}} \\ -\sqrt{\frac{p\tilde{\sigma}}{M}} \end{pmatrix} \chi(s_3) &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{p\tilde{\sigma}}{M}} \\ -\sqrt{\frac{p\sigma}{M}} \end{pmatrix}^{*} \chi(-s_3)(-1)^{s-s_3}, \end{aligned} \tag{5.308}$$

and therefore

$$\begin{aligned} C\gamma_5 u(\mathbf{p}, s_3) &= u^*(-\mathbf{p}, -s_3)(-1)^{s-s_3}, \\ C\gamma_5 v(\mathbf{p}, s_3) &= v^*(-\mathbf{p}, -s_3)(-1)^{s-s_3}, \end{aligned} \tag{5.309}$$

Comparing now the two sides of Eqs. (5.304) we obtain the transformation laws for the creation and annihilation operators

$$\begin{aligned} \mathcal{T} a^{\dagger}_{\mathbf{p},s_3} \mathcal{T}^{-1} \equiv a'^{\dagger}_{\mathbf{p},s_3} &= \eta_T a^{\dagger}_{\mathbf{p},s_3'} c_{s_3' s_3} = \eta_T (-1)^{s-s_3} a^{\dagger}_{-\mathbf{p},-s_3}, \\ \mathcal{T} b^{\dagger}_{\mathbf{p},s_3} \mathcal{T}^{-1} \equiv b'^{\dagger}_{\mathbf{p},s_3} &= \eta_T b^{\dagger}_{\mathbf{p},s_3'} c_{s_3' s_3} = \eta_T (-1)^{s-s_3} b^{\dagger}_{-\mathbf{p},-s_3}. \end{aligned} \tag{5.310}$$

The occurrence of the c-matrix accounts for the fact that the time-reversed state has the opposite internal rotational motion, with the phases adjusted so that the rotation properties of the transformed state remain correct.

The operator $\mathcal{T}$ is antilinear and antiunitary. This has the effect that just as the wave functions of the Schrödinger theory, the Dirac wave function of a particle of momentum $\mathbf{p}$

$$\mathrm{f}_{\mathbf{p}}(x) = u(\mathbf{p}, s_3) e^{-ipx} \tag{5.311}$$

receives a complex conjugation under time reversal:

$$\mathrm{f}_{\mathbf{p},s_3}(x) \xrightarrow{T} \mathrm{f}_{\mathbf{p},s_3\,T}(x) = D(T)\mathrm{f}^{*}_{\mathbf{p},s_3}(x_T) = D(T)u^*(\mathbf{p}, s_3)e^{-i\tilde{p}x} \tag{5.312}$$

The time-reversed wave function on the right-hand side satisfies again the Dirac equation

$$(i\tilde{\not{\partial}} - M)\mathrm{f}_{\mathbf{p},s_3\,T}(x) = 0. \tag{5.313}$$

In momentum space this reads

$$(\not{p} - M)D(T)u^*(-\mathbf{p}, s_3) = 0, \tag{5.314}$$

and this follows directly from (3.564) and a complex conjugation. A similar consideration holds for a wave function

$$\mathrm{f}^{c}_{\mathbf{p},s_3}(x) = v(\mathbf{p}, s_3)e^{ipx}, \tag{5.315}$$

where

$$(\not{p} + M)D(T)v^*(-\mathbf{p}, s_3) = 0, \tag{5.316}$$

As discussed previously on p. 182, parity is maximally violated. On may therefore wonder why the neutron, which may be described by a Dirac spinor as far as its Lorentz transformation properties are concerned, has an extremely small electric dipole moment, for which one presently knows only an upper bound:

$$d_{\rm el} < 11 \times 10^{-26}\, e \cdot {\rm cm}. \tag{5.317}$$

It was Landau who first pointed out that this can be understood as being a consequence of the extremely small violation of time reversal invariance. The electric dipole moment is a vector operator $\mathbf{d} = e\mathbf{x}$ where $\mathbf{x}$ is the distance between the positive and negative centers of charge in the particle. This operator is obviously invariant under time reversal. Now, for a neutron at rest, $\mathbf{d}$ must be proportional to the only other vector operator available, which is the spin operator $\boldsymbol{\sigma}$, i.e.,

$$\mathbf{d} = {\rm const.} \times \boldsymbol{\sigma}. \tag{5.318}$$

But under time reversal, the right-hand side changes its sign, whereas the left-hand side does not. The constant must therefore be zero.[16]

Time reversal invariance ensures that a two-particle scattering amplitude for the process

$$1 + 2 \rightarrow 3 + 4 \tag{5.319}$$

is the same as for the reversed process

$$3 + 4 \rightarrow 1 + 2. \tag{5.320}$$

This will be discussed later in Section 7.7, after having developed a scattering theory. Also other consequences of time reversal invariance can be found there.

5.4 FREE PHOTON FIELD

Let us now discuss the quantization of the electromagnetic field. The classical Lagrangian density is, according to (3.229),

$$\mathcal{L}(x) = \frac{1}{2}[\mathbf{E}^2(x) - \mathbf{B}^2(x)] = -\frac{1}{4}F_{\mu\nu}{}^2(x), \tag{5.321}$$

where $\mathbf{E}(x)$ and $\mathbf{B}(x)$ are electric and magnetic fields, and the Euler-Lagrange equations are

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial[\partial_\mu A^\nu]} = \frac{\partial \mathcal{L}}{\partial A^\nu}, \tag{5.322}$$

i.e.,

$$(g_{\mu\nu}\partial^2 - \partial_\nu\partial_\mu)A^\nu(x) = 0. \tag{5.323}$$

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[16] This argument is due to L.D. Landau, Nucl. Phys. **3**, 127 (1957).

5.4.1 Field Quantization

The spatial components $A^i(x)$ $(i = 1, 2, 3)$ have the canonical momenta

$$\pi_i(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^i(x)} = -F_{0i}(x) = -E^i(x), \tag{5.324}$$

which are just the electric field components. The zeroth component $A^0(x)$, however, poses a problem. Its canonical momentum vanishes identically

$$\pi_0(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^0(x)} = 0, \tag{5.325}$$

since the action does not depend on time derivative of $A^0(x)$. This property of the canonical momentum is a so-called *primary constraint* in Dirac's classification scheme of Hamiltonian systems.[17]. As a consequence, the *Euler-Lagrange equation* for $A^0(x)$

$$\partial_i \frac{\partial \mathcal{L}}{\partial[\partial_i A^0]} = \frac{\partial \mathcal{L}}{\partial A^0}, \tag{5.326}$$

is merely an equation of constraint

$$-\boldsymbol{\nabla}\cdot\mathbf{E}(\mathbf{x}, t) = 0. \tag{5.327}$$

which is Coulomb's law for free fields, the first of the field equations (3.238). This is a so-called *secondary constraint* in Dirac's nomenclature.

We have encountered a vanishing field momentum before in the nonhermitian formulation of the complex nonrelativistic and scalar field theries. There, however, this was an artifact of the complex formulation of the canonical formalism [recall the remarks after Eqs. (5.4.1) and (5.207)], and the field was fully dynamical.

Let us calculate the Hamiltonian density:

$$\mathcal{H} = \sum_{i=1}^{3} \pi_i \dot{A}^i - \mathcal{L} = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2) + \mathbf{E}\cdot\boldsymbol{\nabla}A^0. \tag{5.328}$$

In the Hamiltonian $H = \int d^3x\, \mathcal{H}$, the last term can be integrated by parts, and we find after neglecting a surface term $\int d^3x\, \boldsymbol{\nabla}\cdot(\mathbf{E}\, A^0)(\mathbf{x}, t)$, and enforcing Coulomb's law (5.327):

$$H = \int d^3x\, \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2). \tag{5.329}$$

We now attempt to convert the canonical fields $A^i(\mathbf{x}, t)$ and $E^i(\mathbf{x}, t)$ into field operators by enforcing canonical commutation rules. There is, however, an immediate obstacle to this caused by Coulomb's law. Proceeding straight-forwardly, we would impose the equal-time commutators

$$\left[A^i(\mathbf{x}, t), A^j(\mathbf{x}', t)\right] = 0,$$

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[17] P.A.M. Dirac, *The Principles of Quantum Mechanics*, Oxford University Press, Oxford, Third Edition, 1947, p.114.

$$\begin{aligned}\left[\pi_i(\mathbf{x},t),\pi_j(\mathbf{x}',t)\right] &= 0, \\ \left[\pi_i(\mathbf{x},t),A^j(\mathbf{x}',t)\right] &= -\left[E^i(\mathbf{x},t),A^j(\mathbf{x}',t)\right] = -i\delta^{ij}\delta^{(3)}(\mathbf{x}-\mathbf{x}').\end{aligned} \tag{5.330}$$

But the third equation is incompatible with Coulomb's law (5.327). The reason for this is clear: We have seen above that the zeroth component of the vector potential $A^0(\mathbf{x},t)$ cannot become an operator. But then Coulomb's law, written out as

$$\boldsymbol{\nabla}^2 A^0(\mathbf{x},t) = -\partial^0\, \boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t). \tag{5.331}$$

implies that $\boldsymbol{\nabla}\cdot\mathbf{A}(x)$ cannot be an operator either, and must commute with the canonical field operators $A^i(\mathbf{x},t)$ and $E^i(\mathbf{x},t)$. The commutation with $A^i(\mathbf{x},t)$ follows directly from the first relation (5.330). In order to enforce also the commutation with $E^i(\mathbf{x},t)$, we must correct the canonical commutation rules between $E^i(\mathbf{x},t)$ and $A^j(\mathbf{x}',t)$. Thus we replace the third commutator in (5.330) by

$$\left[\pi_i(\mathbf{x},t),A^j(\mathbf{x}',t)\right] = -\left[E^i(\mathbf{x},t),A^j(\mathbf{x}',t)\right] = -i\delta_T^{ij}(\mathbf{x}-\mathbf{x}'). \tag{5.332}$$

where $\delta_T^{ij}(\mathbf{x}-\mathbf{x}')$ is the *transverse δ-function*

$$\delta_T^{ij}(\mathbf{x}-\mathbf{x}') \equiv \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\left(\delta^{ij}-\frac{k^ik^j}{\mathbf{k}^2}\right). \tag{5.333}$$

By construction, leads to a vanishing commutation rule

$$\left[E^i(\mathbf{x},t),\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x}',t)\right] = 0, \tag{5.334}$$

which ensures that $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x}',t)$ is a *c*-number field, just as $A^0(\mathbf{x}',t)$, thus complying with Coulomb's law (5.331).

In the second-quantized theory, the fields $A^0(\mathbf{x},t)$ and $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)$ play a rather inert role. Both are determined by an equation of motion. The reason for this lies in the gauge invariance of the action, which makes the theory independent of the choice of $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)$, or $A^0(\mathbf{x},t)$. In Section 3.6.2 we have learned that we are free to choose the Coulomb gauge in which $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)$ vanishes identically, so that by (5.331) also $A^0(\mathbf{x},t)\equiv 0$.

In the Coulomb gauge, the canonical field momenta of the vector potential (5.324) are simply their time derivatives:

$$\pi_i(\mathbf{x},t) = -E^i(\mathbf{x},t) = \dot{A}^i(\mathbf{x},t), \tag{5.335}$$

just as for scalar fields [see (5.1)]

We are now ready to expand each component of the vector potential into plane waves just as previously the scalar field

$$A^\mu(x) = \sum_{\mathbf{k},\lambda}\frac{1}{\sqrt{2Vk^0}}\left[e^{-ikx}\epsilon^\mu(\mathbf{k},\lambda)a_{\mathbf{k},\lambda} + \epsilon^{\mu *}(\mathbf{k},\lambda)a^\dagger_{\mathbf{k},\lambda}\right], \tag{5.336}$$

where $\epsilon^{\mu}(\mathbf{k},\lambda)$ are polarization vectors (3.296), (3.308) labeled by $\lambda=\pm1$:

$$\epsilon^{\nu}(\mathbf{k},\lambda)\equiv(0,\boldsymbol{\epsilon}(\mathbf{k},\lambda)),\tag{5.337}$$

with the transverse spatial polarization vectors

$$\boldsymbol{\epsilon}\,(\mathbf{k},\pm1)=\mp\frac{1}{\sqrt{2}}\left(\begin{array}{c}\cos\theta\cos\phi\mp i\sin\phi\\ \cos\theta\sin\phi\pm i\sin\phi\\ -\sin\theta\end{array}\right).\tag{5.338}$$

The four-dimensional polarization vectors (3.296) satisfy the othonormality condition (3.311) and having the polarization sums (3.314) and (3.318) .

Let us quantize the vector field (5.336). In order to impose the canonical commutation rules upon the creation and annihilation operators, we invert the field expansion (5.336) as in the scalar equation (5.14), and find:[18]

$$\left\{\begin{array}{c}a_{\mathbf{k},\lambda}\\ a^{\dagger}_{\mathbf{k},\lambda}\end{array}\right\}=e^{\pm ik^0x^0}\frac{1}{\sqrt{2Vk^0}}\left\{\begin{array}{c}\boldsymbol{\epsilon}^*(\mathbf{k},\lambda)\\ \boldsymbol{\epsilon}\,(\mathbf{k},\lambda)\end{array}\right\}\int d^3x\,e^{\mp i\mathbf{kx}}\left[\pm i\dot{\mathbf{A}}(\mathbf{x},t)+k^0\mathbf{A}(\mathbf{x},t)\right].\tag{5.339}$$

Using now the commutators (5.332), we find

$$[a_{\mathbf{k},\lambda},a_{\mathbf{k}',\lambda'}]=0,\quad [a^{\dagger}_{\mathbf{k},\lambda},a^{\dagger}_{\mathbf{k}',\lambda'}]=0,\tag{5.340}$$

and

$$\begin{aligned}[a_{\mathbf{k},\lambda},a^{\dagger}_{\mathbf{k}',\lambda'}] &= \frac{\sqrt{k^0k'^0}}{2V}\left(\frac{1}{k^0}+\frac{1}{k'^0}\right)e^{i(k^0-k'^0)x_0}\\ &\quad\times\int d^3x\,d^3x'e^{-i(\mathbf{kx}-\mathbf{k}'\mathbf{x}')}\epsilon_i^*(\mathbf{k},\lambda)\epsilon_j(\mathbf{k}',\lambda')\,\delta_T^{ij}(\mathbf{x}-\mathbf{x}').\end{aligned}\tag{5.341}$$

Inserting the finite-volume version of the Fourier representation (5.333) of the transverse δ-function,

$$\delta_T^{ij}(\mathbf{x}-\mathbf{x}')\equiv\frac{1}{V}\sum_{\mathbf{p}}e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')}\left(\delta^{ij}-\frac{p^ip^j}{\mathbf{p}^2}\right).\tag{5.342}$$

the spatial integrations can be done with the result

$$\epsilon_i^*(\mathbf{k},\lambda)\epsilon_j(\mathbf{k}',\lambda')\delta_{\mathbf{k},\mathbf{k}'}\left(\delta^{ij}-k^ik^j/\mathbf{k}^2\right).$$

Due to the transversality condition (3.292), this reduces to

$$\epsilon_i^*(\mathbf{k},\lambda)\epsilon_j(\mathbf{k}',\lambda')\delta^{ij}\delta_{\mathbf{k},\mathbf{k}'}.$$

Using the ortonormality relation (3.310), we therefore obtain

$$[a_{\mathbf{k},\lambda},a^{\dagger}_{\mathbf{k}',\lambda'}]=\delta_{\lambda\lambda'}\delta_{\mathbf{k},\mathbf{k}'}.\tag{5.343}$$

Thus we have found the usual commutation rules for the creation and annihilation operators of the two transversely polarized photons existing for each momentum $\mathbf{k}$.

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[18] The reader is invites to express this in terms of a scalar product in analogy with (5.13).

Energy of Free Photons

We can easily express the field energy (5.329) in terms of the field operators. In the Coulomb gauge with $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)=0$, and $\mathbf{E}(\mathbf{x},t)=-\dot{\mathbf{A}}(\mathbf{x},t)$, the field energy simplifies to

$$H=\int d^3x\,\frac{1}{2}\left(\partial_0 A^i\partial_0 A^i+\boldsymbol{\nabla}A^i\;\cdot\boldsymbol{\nabla}A^i\right) \tag{5.344}$$

This is a sum over the field energies of the three components $A^i(\mathbf{x},t)$, each of them being of the same form as Eq. (5.28) for a scalar field of zero mass. The subsequent calculation is therefore the same as there. Inserting the field expansion (5.336), we find the Hamilton operator

$$H=\sum_{k,\lambda=\pm 1}k^0\left(a^\dagger_{\mathbf{k},\lambda}a_{\mathbf{k},\lambda}+\tfrac{1}{2}\right), \tag{5.345}$$

which contains the vacuum energy

$$E_0\equiv\langle 0|H|0\rangle=\frac{1}{2}\sum_{\mathbf{k},\lambda=\pm 1}k^0=\sum_{\mathbf{k}}\omega_{\mathbf{k}}, \tag{5.346}$$

due to the zero-point oscillations, and counts the energy k^0 of all transverse photons.

Propagator of Free Photons

Let us now calculate the Feynman propagator of the photon field, defined by the vacuum expectation value

$$G^{\mu\nu}(x,x')\equiv\langle 0|TA^\mu(x)A^\nu(x')|0\rangle. \tag{5.347}$$

Inserting the field expansion (5.336), we calculate the vacuum expectation separately for $t>t'$ and $t<t'$ as in (5.44), and find

$$\begin{aligned} G^{\mu\nu}(x,x') &= \Theta(x_0-x_0')\frac{1}{2V}\sum_{\mathbf{k}}\frac{1}{\omega_{\mathbf{k}}}e^{-ik(x-x')}\sum_{\lambda}\epsilon^\mu(\mathbf{k},\lambda)\epsilon^{\nu *}(\mathbf{k},\lambda)\\ &+ \Theta(x_0'-x_0)\frac{1}{2V}\sum_{\mathbf{k}}\frac{1}{\omega_{\mathbf{k}}}e^{ik(x-x')}\sum_{\lambda}\epsilon^{\mu *}(\mathbf{k},\lambda)\epsilon^{\nu *}(\mathbf{k},\lambda). \end{aligned} \tag{5.348}$$

The Heaviside functions are represented as in Eqs. (5.60). The polarization sums in the two terms are real and therefore the same, both being given by the projection matrices $P^{\mu\nu}_{\rm phys}(\mathbf{k})$ or $P^{\mu\nu}_{\rm phys}(k)$ of Eqs. (3.314) or (3.318), respectively Since these are independent of k^0, we may proceed as in going from (5.44) to (5.61), leading to the propagator for in an infinite spatial volume:

$$G^{\mu\nu}(x-x')=\int\frac{d^4k}{(2\pi)^4}e^{-ik(x-x')}\frac{i}{k^2+i\eta}P^{\mu\nu}_{\rm phys}(k). \tag{5.349}$$

The independence of $P^{\mu\nu}_{\rm phys}(k)$ on k^0 permits us assume k^0 in the η-dependent expression (3.318) to be off mass shell, with k^μ following the four-dimensional integration in

(5.349). Alternatively, it may be assumed to be equal to $\mathbf{k}$-dependent the mass-shell value $\omega_{\mathbf{k}}$, i.e., we may use the polarization sum $P^{\mu\nu}_{\rm phys}(\omega_{\mathbf{k}},\mathbf{k})$ rather than (3.318). The latter is, however, an unconventional option, since the off-shell form is more convenient for asessing the consequences of gauge invariance in the presence of charged particles [see the discussion after (10.92)].

For all previous fields, the free-photon propagator was also a Green function of the field equations. Neglecting surface terms, we rewrite the action associated with the Lagrangian density (5.321) after a partial integration as

$$\mathcal{A}=\frac{1}{2}\int d^4x\, A^\mu(x)(g_{\mu\nu}\partial^2-\partial_\mu\partial_\nu)A^\nu(x), \tag{5.350}$$

corresponding to a Lagrangian density

$$\mathcal{L}(x)=\frac{1}{2}A^\mu(x)L_{\mu\nu}(i\partial)A^\nu(x), \tag{5.351}$$

with the differential operator

$$L_{\mu\nu}(i\partial)\equiv g_{\mu\nu}\partial^2-\partial_\mu\partial_\nu. \tag{5.352}$$

The Euler-Lagrange equation (5.323) can then be written simply as

$$L_{\mu\nu}(i\partial)A^\nu(x)=0. \tag{5.353}$$

Ordinarily we would define a Green function by the inhomogenous differential equation

$$L_{\mu\nu}(i\partial)G^{\nu\lambda}(x-x')=i\delta_\mu{}^\lambda\delta^{(4)}(x-x'). \tag{5.354}$$

Here, however, this equation cannot be solved since the Fourier transform of the differential operator $L_{\mu\nu}(i\partial)$ is the 4×4 -matrix

$$L_{\mu\nu}(k)=-g_{\mu\nu}k^2+k_\mu k_\nu, \tag{5.355}$$

and this possesses an eigenvector with eigenvalue zero, the vector k^ν. Thus $L_{\mu\nu}(k)$ cannot have an inverse, and Eq. (5.354) no solution. Instead, the nonzero spatial components of the propagator (5.349) satisfy the transverse equation

$$L_{ij}(i\partial)G^{jk}(x-x')=-i\delta^{ik}_T(\mathbf{x}-\mathbf{x}')\delta(x^0-x'^0). \tag{5.356}$$

and the transversality condition

$$\partial_i G^{ij}(x-x')=0. \tag{5.357}$$

Let us also calculate the commutator from the Feynman propagator according to the rules (5.202). It is most conveniently expressed in terms of the explicitly k^0-independent projection matrix (3.314) as

$$[A^\mu(x),A^\nu(x')]=\int\frac{d^4k}{(2\pi)^4}\epsilon(k^0)\delta(k^2)e^{-ik(x-x')}P^{\mu\nu}_{\rm phys}(\mathbf{k}). \tag{5.358}$$

Since the polarization sum depends only on the spatial momenta, it can be taken out of the integral replacing k_i by $-i\partial_i$, yielding

$$[A^\mu(x), A^\nu(x')] = \left[-g^{\mu\nu} + \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -\partial^i \partial^j / \boldsymbol{\partial}^2 \end{array} \right)^{\mu\nu} \right] C(x-x'), \qquad (5.359)$$

where $C(x-x')$ is the commutator function of the scalar field defined in (5.53) with Fourier representations (5.54), (5.196), and (5.169). Taking the time derivative of one of the fields we find, using the property $\dot{C}(x-x') = -i\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ for $x^0 = x'^0$ of Eq. (5.55), the canonical equal-time commutator

$$[\dot{A}^\mu(\mathbf{x},t), A^\nu(\mathbf{x}',t)] = -i \left[-g^{\mu\nu} + \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -\partial^i \partial^j / \boldsymbol{\partial}^2 \end{array} \right)^{\mu\nu} \right] \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \qquad (5.360)$$

which was the starting point (5.332) of the quantization procedure in the Coulomb gauge with $\mathbf{E}(\mathbf{x},t) = -\dot{\mathbf{A}}(\mathbf{x},t)$.

5.4.2 Covariant Field Quantization

There exists an alternative formalism in which the photon propagator is manifstely covariant. This can, however, be achieved only at the expense of extending the Hilbert space by a nonphysical sector from which the physical subspace is obtained by certain operator conditions. Such an approach can be followed consistently if the interaction does not mix physical states with unphysical ones. As a function of time, physical states must remain physical, i.e., the physical subspace must be invariant under the dynamics of the system.

Gauge transformations modify only the unphysical states. It will turn out that half of them have a negative or zero norm and do not allow for a probabilistic interpretation. This, however, does not cause any problems since the physical subspace is positive definite and dynamically invariant. On it, the second-quantized time evolution operator $U = e^{-iHt}$ is unitary and the completeness sums between physical observables can be restricted to physical states.

The covariant quantization method is based on a modified Lagrangian in which $A^0(x)$ plays no longer a special role, so that every field component $A^\mu(x)$ possesses a canonically conjugate momentum. For this purpose one introduces an auxiliary field $D(x)$, and adds to the original Lagrangian a so-called *gauge-fixing* term[19]

$$\mathcal{L}(x) \quad \rightarrow \quad \mathcal{L}'(x) = \mathcal{L}(x) + \mathcal{L}_{\rm GF}(x) \qquad (5.361)$$

which is defined by

$$\mathcal{L}_{\rm GF}(x) \quad \equiv \quad -D(x)\partial^\mu A_\mu(x) + \frac{\alpha}{2} D^2(x), \qquad \alpha \geq 0. \qquad (5.362)$$

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[19] This modification is due to E. Fermi, Rev. Mod. Phys. *4*, 125 (1932).

Now it is this auxiliary field $D(x)$ which has no canonical momentum:

$$\pi_D(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{D}(x)} \equiv 0, \tag{5.363}$$

so that the Euler-Lagrange equation for $D(x)$ is not a proper equation of motion, but merely a constraint:

$$\alpha D(x) = \partial_\mu A^\mu(x). \tag{5.364}$$

In contrast to the earlier treatment, all four components of the vector potential $A^\mu(x)$ are now dynamical fields and obey a proper equation of motion:

$$\partial^\mu F_{\mu\nu}(x) = \partial^2 A^\mu(x) - \partial^\mu \partial_\nu A^\nu(x) = -\partial_\nu D(x). \tag{5.365}$$

Together with the constraint (5.364), we can write these field equations as

$$\partial^2 A^\mu(x) - \left(1 - \frac{1}{\alpha}\right) \partial^\mu\, \partial_\nu A^\nu(x) = 0. \tag{5.366}$$

From these we may derive, by one more differentiation, a field equation for $D(x)$:

$$\partial^2 D(x) = 0, \tag{5.367}$$

which shows that $D(x)$ is a massless Klein-Gordon field.

If we want to use the new extended Lagrangian for the description of electromagnetism, where the field equations are $\partial^\mu F_{\mu\nu} = 0$, we have to make sure at the end that $D(x)$ is identically zero at all times. With $D(x)$ satisfying the free Klein Gordon equation (5.367), this is guaranteed if $D(x)$ satisfies the initial conditions

$$\begin{aligned} D(\mathbf{x}, t) &\equiv 0, \quad t = t_0, && (5.368)\\ \dot{D}(\mathbf{x}, t) &\equiv 0, \quad t = t_0. && (5.369) \end{aligned}$$

In other words, if the auxiliary field is zero and does not move at some initial time t_0, for example at $t_0 \to -\infty$, it will vanish everywhere at all times. With these initial conditions we can replace the original Lagrangian density by the extended version $\mathcal{L}'(x)$. This has the desired property that all field components $A^\mu(x)$ possess a proper canonically conjugate momentum:

$$\pi_\mu(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^\mu(x)} = -F_{0\mu}(x) - g_{0\mu} D(x). \tag{5.370}$$

Thus, while the spatial field components $A^i(x)$ have the electric fields $-E^i(x)$ as their canonical momenta as before, the new auxiliary field $-D(x)$ plays the role of a canonical momentum to the time component $A^0(x)$. We can now quantize the fields $A^\mu(x)$ and the associate field momenta $(-D(x), -E^i(x))$ by the canonical equal-time commutation rules:

$$\begin{aligned} \left[A^\mu(\mathbf{x}, t), A^\nu(\mathbf{x}', t)\right] &= 0, & \left[E^i(\mathbf{x}, t), A^j(\mathbf{x}', t)\right] &= i\delta^{ij}\delta^{(3)}(\mathbf{x} - \mathbf{x}'),\\ \left[D(\mathbf{x}, t), A^i(\mathbf{x}', t)\right] &= 0, & \left[D(\mathbf{x}, t), A^0(\mathbf{x}', t)\right] &= i\delta^{(3)}(\mathbf{x} - \mathbf{x}'),\\ \left[E^i(\mathbf{x}, t), E^j(\mathbf{x}', t)\right] &= 0, & \left[D(\mathbf{x}, t), E^i(\mathbf{x}', t)\right] &= 0,\\ \left[E^i(\mathbf{x}, t), A^0(\mathbf{x}', t)\right] &= 0, & \left[D(\mathbf{x}, t), D(\mathbf{x}', t)\right] &= 0, && (5.371) \end{aligned}$$

The Hamiltonian density associated with the Lagrangian density $\mathcal{L}'(x)$ is

$$\mathcal{H}'=\pi_\mu\dot{A}^\mu-\mathcal{L}=-\mathbf{E}\cdot\dot{\mathbf{A}}-D\dot{A}^0-\frac{1}{2}(\mathbf{E}^2-\mathbf{B}^2)+D\,\partial^\mu A_\mu-\frac{\alpha}{2}D^2. \tag{5.372}$$

Expressing the electric field in terms of the vector potential, $E^i=-F^{0i}=-\dot{A}^i-\partial_iA^0$, this becomes

$$\mathcal{H}'=\frac{1}{2}\left(\mathbf{E}^2+\mathbf{B}^2\right)+\mathbf{E}\cdot\boldsymbol{\nabla}A^0+D\boldsymbol{\nabla}\cdot\mathbf{A}-\frac{\alpha}{2}D^2. \tag{5.373}$$

For a vanishing field $D(x)$, this is the same Hamiltonian density as before in (5.328).

Let us now quantize this theory in terms of particle creation and annihilation operators.

Feynman Gauge $\alpha=1$

The field equations (5.366) become simplest if we take the special case $\alpha=1$ called the *Feynman gauge*. Then (5.366) reduces to

$$-\partial^2A^\mu(x)=0 \tag{5.374}$$

so that the four components $A^\mu(x)$ simply obey four massless Klein-Gordon equations. The fields can then be expanded into plane-wave solutions as

$$A^\mu(x)=\sum_{\mathbf{k},\nu=0}^{3}\frac{1}{2Vk^0}\left[e^{-ikx}\epsilon^\mu(\nu)a_{\mathbf{k},\nu}+e^{ikx}\epsilon^{\mu*}(\nu)a^\dagger_{\mathbf{k},\nu}\right], \tag{5.375}$$

where $\epsilon^\mu(\nu)$ are now *four* momentum-independent polarization vectors

$$\epsilon^\mu(\nu)=g^{\mu\nu}, \tag{5.376}$$

satisfying the orthogonality and completeness relations

$$\begin{aligned}\epsilon^{\mu*}(\nu)\epsilon_\mu(\nu')&=g_{\nu\nu'}, &(5.377)\\ \sum_{\nu\nu'}g^{\nu\nu'}\epsilon^{\mu'}(\nu)\epsilon^{\nu*}(\nu')&=g^{\mu\nu'}. &(5.378)\end{aligned}$$

Inverting the field expansion, we obtain

$$\left\{\begin{array}{c}a_{\mathbf{k},\nu}\\ a^\dagger_{\mathbf{k},\nu}\end{array}\right\}=e^{\pm ik^0x^0}\sum_{\nu'=0}^{3}g^{\nu\nu'}\frac{1}{\sqrt{2Vk^0}}\left\{\begin{array}{c}\epsilon^*_\mu(\nu')\\ \epsilon_\mu(\nu')\end{array}\right\}\int d^3x\,e^{\pm i\mathbf{kx}}\left[\pm i\dot{A}^\mu(x)+k^0A^\mu(x)\right], \tag{5.379}$$

and are ready to impose canonical commutation rules. From Eqs. (5.371) we see that $A^\mu(\mathbf{x},t)$ and $A^\nu(\mathbf{x},t)$ commute with each other at equal times:

$$[A^\mu(\mathbf{x},t),A^\nu(\mathbf{x}',t)]=0. \tag{5.380}$$

Expressing the canonical momentum (5.370) in terms of the vector potential, $\pi_i(x) = -F_{0i}(x) = -E^i(x) = \dot{A}^i(x) + \partial_i A^0(x)$, the canonical commutator $[\pi_i(\mathbf{x},t), A^j(\mathbf{x}',t)] = -i\delta^{ij}\delta^{(3)}(\mathbf{x}-\mathbf{x}')$ implies

$$[\dot{A}^i(\mathbf{x},t), A^j(\mathbf{x}',t)] = -i\delta_{ij}\delta^{(3)}(\mathbf{x}-\mathbf{x}') - \partial_i[A^0(\mathbf{x},t), A^j(\mathbf{x}',t)]. \tag{5.381}$$

But because of (5.380), we have

$$[\dot{A}^i(\mathbf{x},t), A^j(\mathbf{x}',t)] = -i\delta^{ij}\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{5.382}$$

In contrast to (5.332), the right-hand side is not restricted to the transverse δ-function.

To find the commutation relations for $A^0(\mathbf{x},t)$, we take the canonical commutator

$$[D(\mathbf{x},t), A^0(\mathbf{x}',t)] = i\delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{5.383}$$

and express D in the Feynman gauge as $\partial^\mu A_\mu = \partial_0 A^0 + \partial_i A^i$ [recalling (5.364)]. The commutators of $A^i(x)$ with $A^0(x)$ vanish so that (5.383) amounts to

$$[\dot{A}^0(\mathbf{x},t), A^0(\mathbf{x}',t)] = i\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{5.384}$$

Using the fact that the commutator of $D(\mathbf{x},t)$ with the spatial components $A^i(\mathbf{x}',t)$ vanish by the third of the canonical commutation rules (5.371), the identity (5.364) leads to

$$[\dot{A}^0(\mathbf{x},t), A^i(\mathbf{x}',t)] = 0. \tag{5.385}$$

But one also has

$$[\dot{A}^i(\mathbf{x},t), A^0(\mathbf{x}',t)] = 0. \tag{5.386}$$

This follows from the canonical commutator $[E^i(\mathbf{x},t), A^0(\mathbf{x}',t)] = 0$ after expressing again $E^i = -\dot{A}^i + \partial^i A^0$, or more directly by differentiating the commutator $[A^i(\mathbf{x},t), A^0(\mathbf{x}',t)] = 0$ with respect to t.

For the commutators of the time derivatives of the fields among each other we find similarly

$$\begin{aligned}
\left[\dot{A}^i(\mathbf{x},t), \dot{A}^j(\mathbf{x}',t)\right] &= \left[E^i, E^j\right] + \left\{[E^i, \partial_j A^0] - (ij)\right\} + [\partial_i A^0, \partial_j A^0] = 0,\\
\left[\dot{A}^0(\mathbf{x},t), \dot{A}^i(\mathbf{x}',t)\right] &= \left[D - \partial_j A^j, -E^i - \partial_i A^0\right] = 0,\\
\left[\dot{A}^0(\mathbf{x},t), \dot{A}^0(\mathbf{x}',t)\right] &= \left[D - \partial_j A^j, D - \partial_j A^j\right] = 0.
\end{aligned} \tag{5.387}$$

On the right-hand sides, the equal-time arguments $\mathbf{x}, t$ and $\mathbf{x}', t$ have been omitted, for brevity.

Summarizing, the commutators between the field components $A^\nu(\mathbf{x}',t)$ and their time derivatives are given by the manifestly covariant expressions

$$\begin{aligned}
\left[\dot{A}^\mu(\mathbf{x},t), A^\nu(\mathbf{x}',t)\right] &= ig^{\mu\nu}\delta^{(3)}(\mathbf{x}-\mathbf{x}'),\\
\left[A^\mu(\mathbf{x},t), A^\nu(\mathbf{x}',t)\right] &= 0,\\
\left[\dot{A}^\mu(\mathbf{x},t), \dot{A}^\nu(\mathbf{x}',t)\right] &= 0.
\end{aligned} \tag{5.388}$$

They have the same form as if $A^\mu(\mathbf{x},t)$ were four independent Klein-Gordon fields, except for the fact that the sign in the commutator between the temporal components of $\dot{A}^\mu(\mathbf{x},t)$ is opposite to that between the spatial components. This will be the source of considerable complications in the subsequent discussion.

Using the covariant commutation rules (5.388), we find from (5.379) the commutation rules for the creation and annihilation operators:

$$\begin{aligned} [a_{\mathbf{k},\nu}, a_{\mathbf{k}',\nu'}] &= [a^\dagger_{\mathbf{k},\nu}, a^\dagger_{\mathbf{k}',\nu'}] = 0, \\ [a_{\mathbf{k},\nu}, a^\dagger_{\mathbf{k}',\nu'}] &= -\delta_{\mathbf{k},\mathbf{k}'} g_{\nu\nu'}. \end{aligned} \tag{5.389}$$

It is useful to introduce the contravariant creation and annihilation operators

$$a^{\mu\dagger}_{\mathbf{k}} \equiv \sum_{\nu=0}^{3} \epsilon^{\mu *}(\nu) a^\dagger_{\mathbf{k},\nu}, \qquad a^\mu_{\mathbf{k}} \equiv \sum_{\nu=0}^{3} \epsilon^\mu(\nu) a_{\mathbf{k},\nu}. \tag{5.390}$$

They satisfy the commutation rules

$$\begin{aligned} [a^\mu_{\mathbf{k}}, a^\nu_{\mathbf{k}'}] &= [a^{\mu\dagger}_{\mathbf{k}}, a^{\nu\dagger}_{\mathbf{k}'}] = 0, \\ [a^\mu_{\mathbf{k}}, a^{\nu\dagger}_{\mathbf{k}'}] &= -\delta_{\mathbf{k},\mathbf{k}'} g^{\mu\nu}. \end{aligned} \tag{5.391}$$

The opposite sign of the commutator $[\dot{A}^0(\mathbf{x},t), A^0(\mathbf{x}',t)]$ shows up in the commutators (5.389) and (5.391) between creation and anihilation operators with polarization label $\mu = 0$ or $\nu = 0$. This has the unpleasant consequence that state created by the operators $a^{0\dagger}_{\mathbf{k}} = a^\dagger_{\mathbf{k},0}$ have a negative norm:

$$\langle 0|a^0_{\mathbf{k}} a^{0\dagger}_{\mathbf{k}}|0\rangle \equiv \langle 0|[a^0_{\mathbf{k}}, a^{0\dagger}_{\mathbf{k}}]|0\rangle = -\langle 0|0\rangle = -1. \tag{5.392}$$

Such states cannot be physical. By applying any odd number of these creation operators to the vacuum, one obtains an infinite set of unphysical states.

Another infinite set of unphysical states is

$$|\tilde{0}\rangle_n \equiv (a^{0\dagger}_{\mathbf{k}} \pm a^{3\dagger}_{\mathbf{k}})^n |0\rangle, \qquad n > 1. \tag{5.393}$$

These have a vanishing norm, as follows from the fact that $a^{0\dagger}_{\mathbf{k}} \pm a^{3\dagger}_{\mathbf{k}}$ commutes with its hermitian conjugate. The label 3 can of course be exchanged by 1 or 2.

Fermi-Dirac Subsidiary Condition

At first sight this seems to make the usual probabilistic interpretation of quantum mechanical amplitudes impossible. However, as announced in the beginning, this problem can be circumvented. According to Eqs. (5.365)–(5.369), the classical equations of motion are satisfied correctly only if the auxiliary field $D(x)$ vanishes at some initial time, together with its velocity $\dot{D}(x)$. In the quantized version we have to postulate an equivalent operator property. Exactly the same condition, the vanishing of the second-quantized field operator $D(x)$, would be too stringent: It would contradict the canonical quantization rule

$$[D(\mathbf{x},t), A^0(\mathbf{x}',t)] = i\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{5.394}$$

We can only require that the equation $D(\mathbf{x},t)=0$ is true when applied to physical states. Thus we postulate that only those states in the Hilbert space are physical which satisfy the subsidiary conditions

$$D(\mathbf{x},t)|\psi_{\rm phys}\rangle = 0, \quad \dot{D}(\mathbf{x},t)|\psi_{\rm phys}\rangle = 0 \tag{5.395}$$

at some fixed initial time t. Because of the equation of motion (5.367) for $D(x)$, this is equivalent to requiring

$$D(\mathbf{x},t)|\psi_{\rm phys}\rangle \equiv 0 \tag{5.396}$$

at all times. This is called the *Fermi-Dirac condition.*[20]

In order to discuss its consequences it is useful to introduce the "vectors"

$$\hat{k}_s^\mu \equiv k^\mu/k^0, \quad \hat{k}_l^\mu \equiv \tilde{k}^\mu/2k^0, \quad \text{with} \quad k\equiv(k^0,\mathbf{k}), \quad \tilde{k}\equiv(k^0,-\mathbf{k}). \tag{5.397}$$

and $k^0 = |\mathbf{k}|$ being on the light cone. The quotation marks are used in the same sense as in Section 3.10.7, where we introduced the "vector" (3.387). Due to the normalization factors, both $\hat{k}_s^\mu$ and $\hat{k}_l^\mu$ do *not* transform like vectors under Lorentz transformations. Nevertheless, they do have Lorentz-invariant scalar products with each other:

$$\hat{k}_s\hat{k}_s = 0, \quad \hat{k}_l\hat{k}_l = 0, \quad \hat{k}_s\hat{k}_l = 1. \tag{5.398}$$

In analogy with the (3.345) (3.387), we shall span the four-dimensional vector space here by supplementing the transverse polarization vectors (3.308), (5.337) by the four-component objects

$$\epsilon^\mu(\mathbf{k},s) = \hat{k}_s^\mu, \qquad \epsilon^\mu(\mathbf{k},\bar{s}) = \hat{k}_{\bar{s}}^\mu. \tag{5.399}$$

These agree with the earlier-introduced scalar and antiscalar polarization vectors (3.345) and (3.387) in Section 3.10.7, except for a different normalization which will be more convenient in the sequel. We shall use the same symbols for these new objects, to prevent a proliferation of symbols, in spite of a small danger of confusion. Together with the transverse polarization vectors (3.308), the four "vectors" satisfy the orthogonality relation

$$\epsilon_{\mu *}(\mathbf{k},\sigma)\epsilon^\mu(\mathbf{k},\sigma') = g_{\sigma\sigma'}, \tag{5.400}$$

where the index σ runs through $+1,-1,s,\bar{s}$, and $g_{\sigma\sigma'}$ is the metric

$$g_{\sigma\sigma'} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}_{\sigma\sigma'} \tag{5.401}$$

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[20] E. Fermi, Rev. Mod. Phys. *4*, 87, (1932); P.A.M. Dirac, *Lectures in Quantum Field Theory*, Academic Press, New York, 1966; W. Heisenberg and W. Pauli, Z. Phys. *59*, 168 (1930).

The completeness relation reads, in a slight modification of (3.388),

$$\sum_{\sigma=\pm 1,s,\bar{s}} \epsilon^{\mu}(\mathbf{k},\sigma)\epsilon^{\nu *}(\mathbf{k},\sigma')g^{\sigma\sigma'} = g^{\mu\nu}. \tag{5.402}$$

Multiplying the field expansion (5.375) with the left-hand side of this relation, and defining creation and annihilation operators with polarization label $\sigma = \pm 1, s, \bar{s}$ by

$$a_{\mathbf{k},\sigma} = \epsilon_{\mu}^{*}(\sigma)\sum_{\nu=0}^{3}\epsilon_{\mu}(\nu)a_{\mathbf{k},\nu}, \qquad a_{\mathbf{k},\sigma}^{\dagger} = \epsilon_{\mu}(\sigma)\sum_{\nu=0}^{3}\epsilon_{\mu *}(\nu)a_{\mathbf{k},\nu}^{\dagger}, \tag{5.403}$$

we obtain the new field expansion

$$A^{\mu}(x) = \sum_{\mathbf{k}}\frac{1}{2Vk^{0}}\sum_{\sigma=\pm 1,s,\bar{s}}\left[e^{-ikx}\epsilon^{\mu}(\mathbf{k},\sigma)a_{\mathbf{k},\sigma} + e^{ikx}\epsilon^{\mu *}(\mathbf{k},\sigma)a_{\mathbf{k},\sigma}^{\dagger}\right], \tag{5.404}$$

This expansion may be inverted by euqations like (5.379), expressing the new creation and annihilation operators $a_{\mathbf{k},\sigma}^{\dagger}$ and $a_{\mathbf{k},\sigma}$ in terms of the fields $A^{\mu}(x)$ and $\dot{A}^{\mu}(x)$. The result looks precisely the same as in (5.379), except that the metric $g^{\nu\nu'}$ is replaced by $g^{\sigma\sigma'}$ of (5.401), and the polarization vectors $\epsilon^{\mu}(\nu')$ by $\epsilon^{\mu}(\mathbf{k},\sigma')$.

For the two transverse polarization labels $\sigma = \pm 1$, the new creation and annihilation operators coincide with those introduced during the earlier the noncovariat quantization in expansion (5.336), i.e., the operators $a_{\mathbf{k},\sigma}^{\dagger}$ are equal to $a_{\mathbf{k},\lambda}^{\dagger}$ for polarization labels $\sigma = \lambda = \pm 1$. In addition, the new expansion (5.404) contains the creation and annihilation operators:

$$a_{\mathbf{k},s} = \hat{k}_{s}^{\mu}\sum_{\nu=0}^{3}\epsilon_{\mu}(\nu)a_{\mathbf{k},\nu}, \qquad a_{\mathbf{k},s}^{\dagger} = \hat{k}_{s}^{\mu}\sum_{\nu=0}^{3}\epsilon_{\mu}^{*}(\nu)a_{\mathbf{k},\nu}^{\dagger}, \tag{5.405}$$

$$a_{\mathbf{k},\bar{s}} = \hat{k}_{\bar{s}}^{\mu}\sum_{\nu=0}^{3}\epsilon_{\mu}(\nu)a_{\mathbf{k},\nu}, \qquad a_{\mathbf{k},\bar{s}}^{\dagger} = \hat{k}_{\bar{s}}^{\mu}\sum_{\nu=0}^{3}\epsilon_{\mu}^{*}(\nu)a_{\mathbf{k},\nu}^{\dagger}. \tag{5.406}$$

For the spatial momenta $\mathbf{k}$ pointing in the z-direction, these are

$$\begin{aligned} a_{\mathbf{k},s} &= a_{\mathbf{k}}^{0} - a_{\mathbf{k}}^{3}, \qquad a_{\mathbf{k},s}^{\dagger} = a_{\mathbf{k}}^{0\dagger} - a_{\mathbf{k}}^{3\dagger}, \\ a_{\mathbf{k},\bar{s}} &= a_{\mathbf{k}}^{0} + a_{\mathbf{k}}^{3}, \qquad a_{\mathbf{k},s}^{\dagger} = a_{\mathbf{k}}^{0\dagger} + a_{\mathbf{k}}^{3\dagger}. \end{aligned} \tag{5.407}$$

Note that the previous physical polarization sum (5.388) may be written as

$$P_{\rm phys}^{\mu\nu}(\mathbf{k}) \;=\; \sum_{\sigma=\pm 1}\epsilon^{\mu}(\mathbf{k},\sigma)\epsilon^{\nu}(\mathbf{k},\sigma) = -g^{\mu\nu} + \hat{k}_{s}^{\mu}\hat{k}_{\bar{s}}^{\nu} + \hat{k}_{\bar{s}}^{\mu}\hat{k}_{s}^{\nu}. \tag{5.408}$$

The commutation rules for the new creation and annihilation operators are

$$\begin{aligned} [a_{\mathbf{k},\sigma}, a_{\mathbf{k}',\sigma'}] &= [a_{\mathbf{k},\sigma}^{\dagger}, a_{\mathbf{k}',\sigma'}^{\dagger}] = 0, \\ [a_{\mathbf{k},\sigma}, a_{\mathbf{k},\sigma'}^{\dagger}] &= -g_{\sigma\sigma'}\delta_{\mathbf{k},\mathbf{k}'}. \end{aligned} \tag{5.409}$$

By Fourier-transforming the field $D(x)$, we see that the Fermi-Dirac condition can be rewritten as

$$\begin{aligned} a_{\mathbf{k},s}|\psi_{\rm phys}\rangle &= 0, \qquad (5.410)\\ a^\dagger_{\mathbf{k},s}|\psi_{\rm phys}\rangle &= 0, \qquad (5.411) \end{aligned}$$

i.e., the physical vacuum is annihilated by the *scalar* creation *and* annihilation operators.

Let us calculate the energy of the free-photon system. For this we integrate the Hamiltonian density (5.373) over all space, insert $D(x) = \dot{A}^0(x) + \partial_i A^i(x)$, $\mathbf{E}(x) = --\dot{\mathbf{A}}^i - \boldsymbol{\nabla} A^0$, $\mathbf{B}(x) = \boldsymbol{\nabla}\times\mathbf{A}(\mathbf{x})$, and perform some partial integrations, neglecting surface terms, to obtain for $\alpha = 1$ the simple expression

$$H' = \int d^3x\, \frac{1}{2}(-\dot{A}^\mu \dot{A}_\mu - \boldsymbol{\nabla}A^\mu \boldsymbol{\nabla}A_\mu). \qquad (5.412)$$

This is precisely the sum of four independent Klein-Gordon energies [compare with (5.29) and contrast this with (5.344)], one for each spacetime component $A^\mu(x)$. Due to relativistic invariance, however, the energy of the component $A^0(x)$ has an opposite sign which is related to the above-observed opposite sign in the commutation relations (5.389) and (5.391) for the $\nu = 0$ and $\mu = 0$ polarizations of the creation and annihilation operators.

Inserting now the expansion (5.375) of the field $A^\mu(x)$ in terms of creation and annihilation operators, we obtain by the same calculation which led to Eqs. (5.80) and (5.345):

$$H' = \sum_{\mathbf{k}} \frac{k^0}{2}\left[-a^\dagger_{\mathbf{k},\nu} a_{\mathbf{k},\nu'} - a_{\mathbf{k},\nu} a^\dagger_{\mathbf{k},\nu'}\right] g^{\nu\nu'} = \sum_{\mathbf{k}} \frac{k^0}{2}\left[-a^\dagger_{\mathbf{k},\mu} a^\mu_{\mathbf{k}} - a^\mu_{\mathbf{k}} a^\dagger_{\mathbf{k},\mu}\right]. \qquad (5.413)$$

This operator corresponds to an infinite set of four-dimensional oscillators, one for every spatial momentum and polarization state. Due to the indefinite metric $g^{\nu\nu'}$, the Hilbert space is not of the usual type, and the subsidiary conditions (5.410) and (5.411) are necessary to extract physically consistent results.

The expansion (5.404) in terms of transverse, scalar, and longitudinal creation and annihilation operators yields the Hamiltonian (5.413) in the form

$$H' = \sum_{\mathbf{k}} \frac{k^0}{2}\Big[\sum_{\sigma=\pm1}\left(a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + a_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k},\sigma}\right) - a_{\mathbf{k},s} a^\dagger_{\mathbf{k},\bar{s}} - a_{\mathbf{k},\bar{s}} a^\dagger_{\mathbf{k},s} - a^\dagger_{\mathbf{k},\bar{s}} a_{\mathbf{k},s} - a^\dagger_{\mathbf{k},s} a_{\mathbf{k},\bar{s}}\Big]. \qquad (5.414)$$

Let us bring this operator to *physical normal order*, i.e., to normal order with respect to the physical vacuum. For the transverse modes we move the annihilation operators to the right of the creation operators, as usual. For the modes s and l, the physical normal order has the operators $a_{\mathbf{k},s}$ and $a^\dagger_{\mathbf{k},s}$ on the right to make use of subsidiary conditions (5.410) which are true also for the physical vacuum. Using the two commutation rules

$$\begin{aligned}[][a_{\mathbf{k},\bar{s}}, a^\dagger_{\mathbf{k}',s}] &= -\delta_{\mathbf{k},\mathbf{k}'}, \\ [a^\dagger_{\mathbf{k},\bar{s}}, a_{\mathbf{k}',s}] &= \delta_{\mathbf{k},\mathbf{k}'},\end{aligned} \tag{5.415}$$

the Hamiltonian takes the form:

$$H' = \sum_{\mathbf{k}} k^0 \Big[\sum_{\sigma=\pm 1} \left(a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2} \right) - a_{\mathbf{k},\bar{s}} a^\dagger_{\mathbf{k},s} - a^\dagger_{\mathbf{k},\bar{s}} a_{\mathbf{k},s} \Big]. \tag{5.416}$$

Note that the ordering of the s and l components produces no constant term due to the opposite signs on the right-hand sides of the commutation rules (5.415). The Dirac conditions (5.410) and (5.411) have the consequance that the last two terms vanish for *all* physical states. Thus the Hamilton operator contains only the energies of transverse photons and can be replaced by

$$H'_{\text{phys}} = \sum_{\mathbf{k}} \frac{k^0}{2} \sum_{\sigma=\pm 1} \left(a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + a_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k},\sigma} \right). \tag{5.417}$$

Finally, we bring also the transverse creation and annihilation operators to a normal order (for transverse photons, the ordinary and the physical normal orders are the same), and obtain

$$H'_{\text{phys}} = \sum_{\mathbf{k}} k^0 \sum_{\sigma=\pm 1} \left(a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2} \right). \tag{5.418}$$

The second term gives the vacuum energy:

$$E_0 \equiv \langle 0|H'|0\rangle = \frac{1}{2} \sum_{\mathbf{k}} k^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}}. \tag{5.419}$$

In contrast to all other particles, this divergent expression has immediate experimental consequences in the laboratory — it is observable as the so-called Casimir effect, to be discussed Section 5.10.

The photon number operator obtained by dropping the factor $k^0/2$ in the normally ordered part of the Hamiltonian (5.414):

$$N = \sum_{\mathbf{k}} \Bigg[\Bigg(\sum_{\sigma=\pm 1} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} \Bigg) - a^\dagger_{\mathbf{k},\bar{s}} a_{\mathbf{k},s} - a^\dagger_{\mathbf{k},s} a_{\mathbf{k},\bar{s}} \Bigg] \tag{5.420}$$

With the Dirac conditions (5.410) and (5.411), the last two terms can be omitted between physical states, so that only the transverse photons are counted:

$$N = \sum_{\mathbf{k}} \sum_{\sigma=\pm 1} \left(a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} \right). \tag{5.421}$$

Its action on the physical subspace is completely analogous to that of H'.

Physical Hilbert Space

In the above calculations of the energies we have assumed that the physical vacuum $|0_{\rm phys}\rangle$ has a unit norm. This, however, cannot be true. A simple argument shows that the Fermi-Dirac condition (5.396) is inconsistent with the canonical commutation rule (5.383). For this one considers the diagonal element

$$\langle 0_{\rm phys}|[D(\mathbf{x},t),A^0(\mathbf{x}',t)]|0_{\rm phys}\rangle = i\delta^{(3)}(\mathbf{x}-\mathbf{x}')\langle 0_{\rm phys}|0_{\rm phys}\rangle. \tag{5.422}$$

Writing out the commutator and taking $D(\mathbf{x},t)$ out of the expectation values, the left-hand side apparently vanishes whereas the right-hand side is obviously nonzero. This problem, however, is not fatal for the quantization approach. It occurs and can be solved in ordinary quantum mechanics. Consider the canonical commutator $[p,x]=-i$ between localized states $|x\rangle$:

$$\langle x|[p,x]|x\rangle \overset{\rm not}{=} -i\langle x|x\rangle. \tag{5.423}$$

The left-hand side gives zero, the right-hand side infinity, so the Heisenberg uncertainty principle seems violated. The puzzle is resolved by the fact that Eq. (5.423) is meaningless since the states $|x\rangle$ are not normalizable. The satisfy the orthogonality consition δ-function $\langle x'|x\rangle = \delta(x'-x)$, in which the right-hand side is a distribution. The equation must be multiplied by a smooth test function of x or x' to turn into a finite equation, as in the treatment of Eq. (5.40). Similarly, we can derive from the canonical commutator only the distribution equation

$$\langle x'|[p,x]|x\rangle = -i\langle x'|x\rangle \tag{5.424}$$

with $x \neq x'$, which gives correct finite results after such a smearing procedure.

Another way to escape the contradiction is by abandoning the use of completely localized states $|x\rangle$ and working only with approximately localized states, for example the lattice states $|x^{\rm n}\rangle$ with the proper orthogonality relations (1.173) and completeness relations (1.178). Another possibility is to use a sequence of wave packets in the form of narrow Gaussians

$$\langle x'|x\rangle^\eta = \frac{1}{\sqrt{\pi\eta}}e^{-(x'-x)^2/2\eta} \tag{5.425}$$

which for $\eta \to 0$ becomes more and more localized.

The same subtleties exist for the commutation rule (5.383). The physical states in the Hilbert space are improper states. To see how this comes about let us go to the position representation of the Hamilton operator (5.413) which reads

$$H = \sum_{\mathbf{k}} \frac{k^0}{2}\left[\left(\frac{\partial}{\partial \chi_{\mathbf{k}}}\right)^2 - \chi_{\mathbf{k}}^2\right]. \tag{5.426}$$

where

$$\chi_{\mathbf{k}}^2 = \chi_{\mathbf{k}}^{0\,2} - \chi_{\mathbf{k}}^{1\,2} - \chi_{\mathbf{k}}^{2\,2} - \chi_{\mathbf{k}}^{3\,2}. \tag{5.427}$$

The ground state is given by the product of harmonic wave functions

$$\langle\chi|0\rangle = \prod_{\mathbf{k}} \frac{1}{\pi^{1/4}} e^{\chi_{\mathbf{k}}^2/2}. \tag{5.428}$$

The excited states are obtained by applying to this the creation operators

$$a_{\mathbf{k}}^{\mu\dagger} = \frac{1}{\sqrt{2}}\left(\chi_{\mathbf{k}}^{\mu} + g^{\mu\nu}\frac{\partial}{\partial\chi_{\mathbf{k}}^{\nu}}\right). \tag{5.429}$$

Due to the positive sign of $\chi_{\mathbf{k}}^{0\,0}$ in the ground state (5.428), this procedure does not produce a traditional oscillator Hilbert space with the scalar product

$$\langle\psi'|\psi\rangle = \prod_{\mathbf{k},\mu}\left[\int d\chi_{\mathbf{k}}^{\mu}\right]\langle\psi'|\chi\rangle\langle\chi|\psi\rangle. \tag{5.430}$$

This is not a serious problem, however, since it can be resolved by rotating the contour of integration in $\chi_{\mathbf{k}}^0$ in the complex $\chi_{\mathbf{k}}^0$-plane by 90^0, so that it runs along the imaginary $\chi_{\mathbf{k}}^0$-axis.

We now impose the subsidiary conditions (5.410) and (5.411) upon this Hilbert space. To simplify the discussion we shall consider only the problematic modes with polarization labels 0 and 3 at a fixed momentum **k** in the z-direction, so that the momentum labels can be suppressed,

Then the conditions (5.410) and (5.411) take the simple form

$$(a^0 - a^3)|\psi_{\rm phys}\rangle = 0 \tag{5.431}$$

and

$$(a^{0\dagger} - a^{3\dagger})|\psi_{\rm phys}\rangle = 0. \tag{5.432}$$

In the position representation, these conditions amount to

$$\begin{aligned}\left(\frac{\partial}{\partial\chi^0} + \frac{\partial}{\partial\chi^3}\right)\langle\chi|\psi_{\rm phys}\rangle &= 0, & (5.433)\\ (\chi_0 - \chi_3)\langle\chi|\psi_{\rm phys}\rangle &= 0. & (5.434)\end{aligned}$$

The first condition is fulfilled by wave functions which do not depend on $\chi^0 + \chi^3$, the second restricts the dependence on $\chi^0 - \chi^3$ to a δ-function. The wave function of the physical vacuum is therefore (for particles of a fixed momentum running along the z-axis)

$$\langle\chi|0_{\rm phys}\rangle = \delta(\chi^0 - \chi^3)\frac{1}{\pi^{1/4}}e^{-(\chi^{1\,2}+\chi^{2\,2})/2}. \tag{5.435}$$

The complete set of physical states is obtained by applying to this any number of creation operators for transverse photons

$$a^{1\dagger} = \frac{1}{\sqrt{2}}\left(\chi^1 - \frac{\partial}{\partial\chi^1}\right), \qquad a^{2\dagger} = \frac{1}{\sqrt{2}}\left(\chi^2 - \frac{\partial}{\partial\chi^2}\right). \tag{5.436}$$

The physical vacuum (5.435) displays precisely the unpleasant feature which caused the problems with the quantum mechanical equation (5.423). Due to the presence of the δ-functions the wave function is *not* normalizable, but a distribution. The normalization problem of the wave function $\delta(\chi^0 - \chi^3)$ is completely analogous to that of ordinary plane waves, and we know how to do quantum mechanics with such generalized states. The standard Hilbert space is obtained by superimposing plane waves to wave packets. Normalizable wave packets can be constructed to approximate the positional wave functions $\delta(\chi^0 - \chi^0)$ in various ways. One may, for instance, discretize the field variables χ^μ and work on a lattice in field space. Alternatively one may replace the δ-function in (5.435) by a narrow Gaussian

$$\delta(\chi^0 - \chi^3) \to \text{const} \times e^{-(\chi^0-\chi^3)^2/2\eta}, \tag{5.437}$$

with an appropriate normalization factor.

When performing calculations in the physical Hilbert space of the Dirac quantization scheme, we would like to proceed as in the case of Klein-Gordon and Dirac particles, assuming that the scalar product $\langle 0_{\rm phys}|0_{\rm phys}\rangle$ is unity, as we did when evaluating the vacuum energy (5.419) (which was really illegal as we have just learned). Only with a unit norm of the vacuum state can we find physical expectation values by simply bringing all creation and annihilation operators between the vacuum states to physical normal order, the desired result being the sum of the c-numbers produced by the commutators. Such a unit norm is achieved by introducing the analogs of the wave packets (5.425), which in the this case are normalizable *would-be vacuum states* to be denoted by $|0_{\rm phys}\rangle^\eta$ which approach the true unnormalizabel vacuum state arbitrarily close for $\eta \to 0$. These would-be vacuum states are most easily constructed algebraically.[21] Considering only the problematic creation and annihilation operators $a^{0\dagger}$, a^0 and $a^{3\dagger}$, a^3, we define an auxiliary state $|0_{\rm aux}\rangle$ to be the one that is annihilated by $a^{0\dagger}$ and a^3:

$$a^{0\dagger}|0_{\rm aux}\rangle = 0, \qquad a^3|0_{\rm aux}\rangle = 0. \tag{5.438}$$

From this we construct the physical vacuum state as a power series

$$|0_{\rm phys}\rangle = \sum_{n,m=0}^{\infty} c_{n,m}(a^{3\dagger})^n(a^0)^m|0_{\rm aux}\rangle. \tag{5.439}$$

The subsidiary conditions (5.410) and (5.411) are now

$$a_s|0_{\rm phys}\rangle = (a^0 - a^3)|0_{\rm phys}\rangle = 0, \qquad a_s^\dagger|0_{\rm phys}\rangle = (a^{0\dagger} - a^{3\dagger})|0_{\rm phys}\rangle = 0. \tag{5.440}$$

These are obviously fulfilled by the *coherent state*:

$$|0_{\rm phys}\rangle = e^{a^{3\dagger}a^0}|0_{\rm aux}\rangle. \tag{5.441}$$

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[21] R. Utiyama, T. Imamura, S. Sunakawa, and T. Dodo, Progr. Theor. Phys. *6*, 587 (1951).

To verify this we merely note that a^3 acts on this state like a differential operator $\partial/\partial a^{3\dagger}$ producing a factor a^0, and the same thing holds with $a^{3\dagger}$ and a^3 replaced by $a^{0\dagger}$ and a^0, respectively.

The norm of this state is infinite:

$$\langle 0_{\rm phys}|0_{\rm phys}\rangle = \sum_{n,m=0}^{\infty}\frac{1}{n!m!}\langle 0_{\rm aux}|(a^3)^n(a^{0\dagger})^n(a^{3\dagger})^m(a^0)^m|0_{\rm aux}\rangle = \sum_{n=0}^{\infty}1=\infty. \tag{5.442}$$

We now approximate this physical vacuum by a sequence of normalized states $|0_{\rm phys}\rangle^\eta$ defined by

$$|0_{\rm phys}\rangle^\eta \equiv \sqrt{\eta(2-\eta)}e^{(1-\eta)a^{3\dagger}a^0} = \sqrt{\eta(2-\eta)}\sum_{n=0}^{\infty}\frac{1}{n!}[(1-\eta)a^{3\dagger}a^0]^n|0_{\rm aux}\rangle. \tag{5.443}$$

It is easy to check that these have a unit norm:

$${}^\eta\langle 0_{\rm phys}|0_{\rm phys}\rangle^\eta = \eta(2-\eta)\sum_{n=0}^{\infty}(1-\eta)^{2n}=1. \tag{5.444}$$

On this sequence of states, the subsidiary conditions (5.440) are not exactly satisfied. Using the above derivative rules, we see that

$$\begin{aligned} a^3|0_{\rm phys}\rangle^\eta &= \frac{\partial}{\partial a^{3\dagger}}|0_{\rm phys}\rangle^\eta = (1-\eta)\,a^0|0_{\rm phys}\rangle^\eta,\\ a^{0\dagger}|0_{\rm phys}\rangle^\eta &= \frac{\partial}{\partial a^0}|0_{\rm phys}\rangle^\eta = (1-\eta)\,a^{3\dagger}|0_{\rm phys}\rangle^\eta, \end{aligned} \tag{5.445}$$

corresponding to the approximate subsidiary conditions

$$\begin{aligned} a_s|0_{\rm phys}\rangle^\eta &= \eta\, a^0|0_{\rm phys}\rangle^\eta,\\ a_s^\dagger|0_{\rm phys}\rangle^\eta &= \eta\, a^{3\dagger}|0_{\rm phys}\rangle^\eta. \end{aligned} \tag{5.446}$$

Let us calculate the norm of the states on the rigth-hand side. Using the power series expansion (5.443) we find

$$\begin{aligned} &{}^\eta\langle 0_{\rm phys}|a^3a^{3\dagger}|0_{\rm phys}\rangle^\eta\\ &\quad= \eta(2-\eta)\sum_{n,m=0}^{\infty}\frac{1}{n!m!}\langle 0_{\rm aux}|(1-\eta)^n(a^3)^n(a^{0\dagger})^n\,a^3a^{3\dagger}\,(1-\eta)^m(a^{3\dagger})^m(a^0)^m|0_{\rm aux}\rangle\\ &\quad= \eta(2-\eta)\sum_{n=0}^{\infty}(n+1)(1-\eta)^{2n}, \end{aligned} \tag{5.447}$$

and thus

$${}^\eta\langle 0_{\rm phys}|a^3a^{3\dagger}|0_{\rm phys}\rangle^\eta = \frac{1}{\eta(2-\eta)}. \tag{5.448}$$

Similarly we derive

$$ {}^{\eta}\langle 0_{\rm phys}|a^{0\dagger}a^{0}|0_{\rm phys}\rangle^{\eta} = \frac{1}{\eta(2-\eta)}, \tag{5.449}$$

and via the commutation rules

$$ a^0a^{0\dagger} = -1 + a^{0\dagger}a^0, \qquad a^{3\dagger}a^3 = -1 + a^3a^{3\dagger}, \tag{5.450}$$

the expectation values

$$ {}^{\eta}\langle 0_{\rm phys}|a^{0}a^{0\dagger}|0_{\rm phys}\rangle^{\eta} = {}^{\eta}\langle 0_{\rm phys}|a^{3\dagger}a^{3}|0_{\rm phys}\rangle^{\eta} = \frac{(1-\eta)^2}{\eta(2-\eta)}, \tag{5.451}$$

These results can actually be obtained by trivial algebra directly from Eqs. (5.446) using the commutation relations (5.450).

Equations (5.448) and (5.449) show that the norm of the states on the right-hand side of Eqs. (5.446) is $\sqrt{\eta/(1-\eta)}$, the normalized states $|0_{\rm phys}\rangle^{\eta}$ satisfy the desired constraints (5.440) in the limit $\eta \to 0$, thus converging towards the physical vacuum state.

To be consistent, all calculations in the Dirac quantization scheme have to be done in one of the would-be vacuum states $|0_{\rm phys}\rangle^{\eta}$, with the limit taken at the end. Only in this way, the earlier-observed apparent contradiction (5.422) and (5.423) can be avoided. In the present context, it is observed when taking the expectation value of the commutation relation $[a_{\bar s}, a_s^\dagger] = -1$:

$$ \langle 0_{\rm phys}|a_{\bar s}a_s^{\dagger}|0_{\rm phys}\rangle - \langle 0_{\rm phys}|a_s^{\dagger}a_{\bar s}|0_{\rm phys}\rangle = -\langle 0_{\rm phys}|0_{\rm phys}\rangle. \tag{5.452}$$

Since $a_s^\dagger$ annihilates the physical vacuum to its right and to its left, the left-hand side should be zero, contradicting the right-hand side. For the normalized finite-η would-be vacuum, on the other hand, the equation becomes

$$ {}^{\eta}\langle 0_{\rm phys}|a_{\bar s}a_s^{\dagger}|0_{\rm phys}\rangle^{\eta} - {}^{\eta}\langle 0_{\rm phys}|a_s^{\dagger}a_{\bar s}|0_{\rm phys}\rangle^{\eta} = -1. \tag{5.453}$$

From (5.448)–(5.449) we find

$$ {}^{\eta}\langle 0_{\rm phys}|a_{\bar s}a_s^{\dagger}|0_{\rm phys}\rangle^{\eta} = -1, \qquad {}^{\eta}\langle 0_{\rm phys}|a_s^{\dagger}a_{\bar s}|0_{\rm phys}\rangle^{\eta} = -1, \tag{5.454}$$

so that (5.453) is a correct equation. Thus, although the states (5.446) have a small norm of order $\sqrt{\eta}$, the products $a_{\bar s}a_s^\dagger$ and $a_s^\dagger a_{\bar s}$ have a unit expectation value.

We can easily see the reason for this by calculating

$$\begin{aligned} a_{\bar s}|0_{\rm phys}\rangle^{\eta} &= (2-\eta)\,a^0|0_{\rm phys}\rangle^{\eta}, \\ a_{\bar s}^{\dagger}|0_{\rm phys}\rangle^{\eta} &= (2-\eta)\,a^{3\dagger}|0_{\rm phys}\rangle^{\eta}, \end{aligned} \tag{5.455}$$

and observing that the norm of the states on the right-hand sides is, by (5.448) and (5.449), equal to $(2-\eta)/\sqrt{\eta(2-\eta)} = \sqrt{(2-\eta)/\eta}$, which diverges like $1/\sqrt{\eta}$ for

$\eta \to 0$ [being precisely the inverse of the norm of the states (5.446)]. Thus we can only drop safely expectation values in which a_s or $a_s^\dagger$ act upon the physical vacuum to its right, if there is no operator $a_{\bar{s}}^\dagger$ or $a_{\bar{s}}$ doing the same thing to its left. This could be a problem with respect to the vacuum energy of the unphysical modes in (5.414), which is proportional to

$$-\,^\eta\langle 0_{\rm phys}|a_s a_{\bar{s}}^\dagger + a_{\bar{s}} a_s^\dagger + a_{\bar{s}}^\dagger a_s + a_s^\dagger a_{\bar{s}}|0_{\rm phys}\rangle^\eta. \tag{5.456}$$

Fortunately, this expectation value does vanish, as it should, since by (5.448)–(5.451):

$$\begin{aligned} ^\eta\langle 0_{\rm phys}|a_s a_{\bar{s}}^\dagger|0_{\rm phys}\rangle^\eta &= {}^\eta\langle 0_{\rm phys}|a_{\bar{s}} a_s^\dagger|0_{\rm phys}\rangle^\eta = 1/2, \\ ^\eta\langle 0_{\rm phys}|a_s^\dagger a_{\bar{s}}|0_{\rm phys}\rangle^\eta &= {}^\eta\langle 0_{\rm phys}|a_{\bar{s}}^\dagger a_s|0_{\rm phys}\rangle^\eta = -1/2, \end{aligned} \tag{5.457}$$

so that the energy of the unphysical modes in the normalized would-be vacuum state $|0_{\rm phys}\rangle^\eta$ is indeed zero for all η, and the true vacuum energy in the limit $\eta \to 0$ contains only the zero-point oscillations of the physical transverse modes.

In this context it is worth emphasizing that the normally ordered operator $a^{0\dagger}a^0 - a^{3\dagger}a^3$ is *not* normally ordered with respect to the physical vacuum $|0_{\rm phys}\rangle$ and thus does not yield zero when sandwiched between two such states. This is obvious by rewriting $a^{0\dagger}a^0 - a^{3\dagger}a^3$ as $a_{\bar{s}}^\dagger a_s + a_s^\dagger a_{\bar{s}}$, and the fact that the annihilation operator $a_{\bar{s}}$ on the right-hand side do *not* annihilate the physical vacuum: $a_{\mathbf{k},\bar{s}}|0_{\rm phys}\rangle \neq 0$.

In axiomatic quantum field theory, the vacuum is always *postulated* to be a proper discrete state with a unit norm. Without this properties, the discussion of symmetry operations in a Hilbert space becomes quite subtle, since infinitesimal transformations can produce finite changes of a state. The Dirac vacuum $|0_{\rm phys}\rangle$ is not permitted by this postulate, whereas the pseudophysical vacuum $|0_{\rm phys'}\rangle$ is. There are other problems within axiomatic quantum field theory, however, due to the nonuniqueness of this vauum, and due to the fact that the vacuum is not separated from all other states by an energy gap, an important additional postulate. That latter postulate is actually unphysical, due to the masslessness of the photon and the existence of many other massless particles in nature. But it is necessary for the derivation of many "rigorous results" in that somewhat esoteric discipline.

Because of the subtleties with the limiting procedure of the vacuum state, it will not be convenient to work with the Dirac quantization scheme but use a simplified procedure due to Gupta and Bleuler to be introduced below. First, however, we shall complete the present discussion by calculating the photon propagator within the Dirac scheme.

Propagator in Dirac Quantization Scheme

Let us calculate the propagator of the A_μ-field in the Dirac quantization scheme. We take the expansion of the field operator (5.404) and evaluate the expectation value

$$G^{\mu\nu}(x,x') = {}^\eta\langle 0_{\rm phys}|TA^\mu(x)A^\nu(x')|0_{\rm phys}\rangle^\eta, \tag{5.458}$$

letting $\eta \to 0$ at the end. For $x_0 > x_0'$, we obtain a contribution proportional to

$$\Theta(x_0 - x_0')\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}e^{-ik(x-x')} \tag{5.459}$$

multiplied by the sum of the expectation values of

$$\epsilon^{\mu *}(\mathbf{k},+1)\epsilon^{\nu}(\mathbf{k},+1)a_{\mathbf{k},+1}a^{\dagger}_{\mathbf{k},+1}, \qquad \epsilon^{\mu *}(\mathbf{k},-1)\epsilon^{\nu}(\mathbf{k},-1)a_{\mathbf{k},-1}a^{\dagger}_{\mathbf{k},-1}, \tag{5.460}$$

and

$$\epsilon^{\mu *}(\mathbf{k},\bar{s})\epsilon^{\nu}(\mathbf{k},s)a_{\mathbf{k},s}a^{\dagger}_{\mathbf{k},\bar{s}}, \qquad \epsilon^{\mu *}(\mathbf{k},s)\epsilon^{\nu}(\mathbf{k},\bar{s})a_{\mathbf{k},\bar{s}}a^{\dagger}_{\mathbf{k},s}, \tag{5.461}$$

and a contribution proportional to

$$\Theta(x_0 - x_0')\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}e^{ik(x-x')} \tag{5.462}$$

multiplied by the sum of the expectation values of

$$\epsilon^{\mu}(\mathbf{k},+1)\epsilon^{\nu *}(\mathbf{k},+1)a^{\dagger}_{\mathbf{k},+1}a_{\mathbf{k},+1}, \qquad \epsilon^{\mu}(\mathbf{k},-1)\epsilon^{\nu *}(\mathbf{k},-1)a^{\dagger}_{\mathbf{k},-1}a_{\mathbf{k},-1}, \tag{5.463}$$

and

$$\epsilon^{\mu}(\mathbf{k},\bar{s})\epsilon^{\nu *}(\mathbf{k},s)a^{\dagger}_{\mathbf{k},s}a_{\mathbf{k},\bar{s}}, \qquad \epsilon^{\mu}(\mathbf{k},s)\epsilon^{\nu *}(\mathbf{k},\bar{s})a^{\dagger}_{\mathbf{k},\bar{s}}a_{\mathbf{k},s}. \tag{5.464}$$

The first two terms containing transverse photons produce a polarization sum

$$\epsilon^{\mu *}(\mathbf{k},+1)\epsilon^{\nu}(\mathbf{k},+1) + \epsilon^{\mu *}(\mathbf{k},-1)\epsilon^{\nu}(\mathbf{k},-1) \tag{5.465}$$

The expectation values of the normally ordered transverse photon terms (5.463) vanish. The remaining terms in (5.461) and (5.464) are evaluated with the help of the matrix elements (5.457) of opposite signs, and cancel each other, due to the evenness of $\epsilon^{\mu}(\mathbf{k},s)\epsilon^{\nu *}(\mathbf{k},\bar{s}) = {k^0}^2 - {k^3}^2$ functions of k^{μ}. Such a function as a factor inside the momentum sums (5.459) and (5.462) preserves their equality, thus ensuring the cancelation of the contributions from (5.461) and (5.464).

For $x_0 < x_0'$, we obtain once more the same expression with spacetime and Lorentz indices interchanged: $x \leftrightarrow x'$, $\mu \leftrightarrow \nu$.

The propagator becomes therefore

$$\begin{aligned} G^{\mu\nu}(x,x') &= {}^{\eta}\langle 0_{\rm phys}|TA^{\mu}(x)A^{\nu}(x')|0_{\rm phys}\rangle^{\eta} \\ &= \Theta(x_0 - x_0')\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}e^{-ik(x-x')}\sum_{\nu=1}^{2}\epsilon^{\mu *}(\mathbf{k},\nu)\epsilon^{\nu}(\mathbf{k},\nu) \\ &+ \Theta(x_0' - x_0)\frac{1}{V}\sum_{k}\frac{1}{2k^0}e^{ik(x-x')}\sum_{\nu=1}^{2}\epsilon^{\mu *}(\mathbf{k},\nu)\epsilon^{\nu}(\mathbf{k},\nu). \end{aligned} \tag{5.466}$$

This is the same propagator as in Eq. (5.349), where it was obtained in the manifestly noncovariant quantization scheme, in which only the physical degrees of freedom of the vector potential were made operators. Thus, although the field operators have been quantized with the covariant commutation relations (5.371), the selection procedure of the physical states has produced the same noncovariant propagator.

It is worth pointing out the difference between the propagator (5.349) and the retarded propagator used in classical electrodynamics. The classical one is given by same Fourier integral as $G(x-x')$:

$$G_R(x-x') \equiv \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-x')} \frac{i}{k^2}, \tag{5.467}$$

except that the poles at $k^0 \equiv \pm\omega = |\mathbf{k}|$ are both placed *below* the real axis. The quantum-field-theoretic k^0-integral

$$\begin{aligned}\int \frac{dk^0}{2\pi} e^{-ik^0(x^0-x'^0)} \frac{i}{2|\mathbf{k}|}\left(\frac{1}{k^0-|\mathbf{k}|+i\eta} - \frac{1}{k^0+|\mathbf{k}|-i\eta}\right) \\ = \frac{1}{2\omega}[\Theta(x^0-x'^0)e^{-i\omega(x^0-x'^0)} + \Theta(x'^0-x^0)e^{i\omega(x^0-x'^0)}] = \frac{1}{2\omega}e^{-i\omega|x^0-x'^0|}\end{aligned} \tag{5.468}$$

with ω on the light cone, $\omega = |\mathbf{k}|$, is to be compared with the retarded expression

$$\begin{aligned}\int \frac{dk^0}{2\pi} e^{-ik^0(x^0-x'^0)} \frac{i}{2|\mathbf{k}|}\left(\frac{1}{k^0-|\mathbf{k}|+i\eta} - \frac{1}{k^0+|\mathbf{k}|+i\eta}\right) \\ = \Theta(x^0-x'^0)\frac{1}{2\omega}(e^{-i\omega(x^0-x'^0)} - e^{i\omega(x^0-x'^0)}) = -2i\Theta(x^0-x'^0)\frac{1}{2\omega}\sin[\omega(x^0-x'^0)].\end{aligned} \tag{5.469}$$

The angular part of the spatial integral

$$\int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{kx}} \tag{5.470}$$

can be done inneither case in the same way leading to

$$\frac{1}{2\pi^2 R}\int_0^\infty d\omega \sin(\omega R). \tag{5.471}$$

Thus we find

$$G_R(x-x') = i\Theta(x^0-x'^0)\int_{-\infty}^{\infty} d\omega\{e^{-i\omega[(x^0-x'^0)-R]} - e^{-i\omega[(x^0-x'^0)+R]}\} \tag{5.472}$$

Since R and $x^0 - x'^0$ are both positive, the result is

$$G_R(x-x') = i\Theta(x^0-x'^0)\frac{1}{4\pi R}\delta(x^0-x'^0-R). \tag{5.473}$$

The retarded propagator exists only for causal times $x^0 > x'^0$ and it is equal to the Coulomb potential if the end points can be connected by a light signal. In contrast to this, the propagator of the quantized electromagnetic field, in which the creation operator of antiparticles accompanies the negative energy solutions of the wave equation, is

$$G(x-x')=i\frac{1}{4\pi R}\delta_+(|x^0-x'^0|-R)+i\frac{1}{4\pi R}\delta_+(-|x^0-x'^0|-R). \tag{5.474}$$

where

$$\delta_+(t)=\int\frac{d\omega}{\pi}e^{-i\omega t} \tag{5.475}$$

is equal to twice the positive-frequency part of Fourier decomposition of the δ-function. With the help of an infinitesimal imaginary part in the time argument, the integral can be done and gives

$$\delta_+(t)=\frac{1}{\pi i}\frac{1}{t-i\eta}. \tag{5.476}$$

This can be decomposed as follows:

$$\delta_+(t)=\frac{1}{\pi i}\left(\frac{i\eta}{t^2+\eta^2}+\frac{t}{t+\eta^2}\right)=\delta(t)+\frac{1}{\pi i}\frac{\mathcal{P}}{t}. \tag{5.477}$$

The second term selects in any integral involving $\delta_+(t)$ the principal value. Note that $\delta_+(t)$ shares with $\delta(t)$ the property

$$\delta(t^2-R^2)=\frac{1}{2R}[\delta(t-R)+\delta(t+R)]. \tag{5.478}$$

Thus the propagator $G(x-x')$ can therefore also be written as

$$G(x-x')=i\frac{1}{2\pi}\delta_+((x-x')^2). \tag{5.479}$$

to be compared with the retarded propagator

$$G_R(x-x')=\Theta(x^0-x'^0)i\frac{1}{2\pi}\delta((x-x')^2). \tag{5.480}$$

The massive propagators in configuration space are, incidentally, quite simply related to the massless ones. One simply writes the δ-functions $\delta((x-x')^2)$ and $\delta_+((x-x')^2)$ and in $G_R(x-x')$ and $G(x-x')$ as Fourier integrals

$$\delta((x-x')^2)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{\omega i(x-x')^2},\quad \delta_+((x-x')^2)=\int_0^{\infty}\frac{d\omega}{\pi}e^{\omega i(x-x')^2} \tag{5.481}$$

and replaces $e^{-i\omega(x-x')^2}$ by $e^{-i\omega(x-x')^2-\frac{M^2}{2\omega}}$ as in (5.131). With this additional term in the exponent, the ω-integrals yield Bessel functions:

$$\begin{aligned}\delta(x^2)&\rightarrow\delta(x^2)+\Theta(x^2)\frac{M^2}{2}\frac{J_1(M\sqrt{x^2})}{M\sqrt{x^2}}, &(5.482)\\ \delta_+(x^2)&\rightarrow\delta(x^2)+\mathcal{P}\frac{M^2}{2}\frac{J_1(M\sqrt{x^2})-iN_1(M\sqrt{x^2})}{M\sqrt{x^2}}. &(5.483)\end{aligned}$$

For $M \to 0$ we use the limiting behavior $J_1(z) \to z/2$, $N_1(z) \to -2/\pi z$ and see that in the first equation the mass term disappears whereas in the second term it yields $\mathcal{P}/\pi i x^2$. The polarization vectors have to satisfy

$$k^2\epsilon^\mu(\mathbf{k},\nu) - \left(1-\frac{1}{\alpha}\right) k^\mu k_\nu \epsilon^\nu(\mathbf{k},\nu) = 0. \tag{5.484}$$

The propagator of the fields A^μ in momentum space is obtained by inverting the inhomogeneous version of this equation: Correspondingly, the polarization vectors in the field expansion (5.375) solutions will now, instead of (5.377)–(5.378), satisfy the completeness and orthogonality relations

$$\begin{aligned} \sum_{\nu\nu'} g^{\nu\nu'}\epsilon^\mu(\mathbf{k},\nu)\epsilon^{\mu'*}(\mathbf{k},\nu') &= g^{\mu\mu'} - (1-\alpha)\frac{k^\mu k^{\mu'}}{k^2}, & (5.485)\\ \left(g^{\mu\mu'} - (1-\alpha)\frac{k^\mu k^{\mu'}}{k^2}\right)\epsilon_{\mu*}(\mathbf{k},\nu)\epsilon_{\mu'}(\mathbf{k},\nu') &= g^{\nu\nu'}. & (5.486) \end{aligned}$$

Gupta-Bleuler Subsidiary Condition

One may wonder whether it is possible to avoid the awesome limiting procedure $\eta \to 0$ and find a way of working with an ordinary vacuum state. This is indeed possible if one is only interested in physical matrix elements containing at least one particle. Such matrix elements can be calculated using only the condition (5.410), while discarding the condition (5.411). Thus, we select what we shall call *pseudo-physical states* by requiring only

$$a_{\mathbf{k},s}|\psi_{\text{“phys”}}\rangle = 0. \tag{5.487}$$

The restriction to this condition is the basis of the *Gupta-Bleuler approach*[22] to quantum electrodynamics. Take, for instance, the number operator (5.420) and insert it between two pseudo-physical states selected in this way. It yields

$$\begin{aligned} \langle\psi'_{\text{“phys”}}|N|\psi_{\text{“phys”}}\rangle &= \langle\psi'_{\text{“phys”}}|a^\dagger_{\mathbf{k},+1}a_{\mathbf{k},+1} + a^\dagger_{\mathbf{k},-1}a_{\mathbf{k},-1}|\psi_{\text{“phys”}}\rangle\\ &\quad -\langle\psi'_{\text{“phys”}}|[a^\dagger_{\mathbf{k},\bar{s}}a_{\mathbf{k},s} + a^\dagger_{\mathbf{k},s}a_{\mathbf{k},\bar{s}}]|\psi_{\text{“phys”}}\rangle. \qquad (5.488) \end{aligned}$$

The second line vanishes because due to the condition (5.433) and its Hermitian adjoint. Thus the number operator counts only the number of transverse photons.

The same mechanism ensures correct particle energies. We bring the Hamilton operator (5.416) with the help of the first commutation rule in (5.415) to the normally ordered form in the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$

$$H' = \sum_{\mathbf{k}} k^0\left[\sum_{\sigma=\pm1}\left(a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} + \frac{1}{2}\right) + 1 - a^\dagger_{\mathbf{k},s}a_{\mathbf{k},\bar{s}} - a^\dagger_{\mathbf{k},\bar{s}}a_{\mathbf{k},s}\right]. \tag{5.489}$$

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[22] K. Bleuler, Helv. Phys. cta *23*, 567 (1950), S.N. Gupta, Proc. Phys. Soc. (London) A *63*, 681 (1950); A *64*, 426 (1951); Phys. Rev. *77*, 294L (1950); *117*, 1146 (1960). For a recent discussion see L.P. Prokhorov, Usp. Fiz. Nauk. *154*, 299 (1988) [transl. in Sov. Phys. Usp. *31*, 151 (1988).

and see that the last two terms vanish because of the Gupta-Bleuler condition (5.487). Thus the Hamilton operator counts only the energies of the transverse photons.

So why did we have to impose the second Dirac condition (5.411) at all? It is needed to ensure only one property of the theory: the correct vacuum energy. In the Gupta-Bleuler approach this energy comes out wrong by a factor two showing that the unphysical degrees of freedom have not been completely eliminated. The normal ordering of the Hamilton operator (5.416) with respect to the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$ has produced an extra vacuum energy

$$E_0^{\text{extra}} = \sum_{\mathbf{k}} k^0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}}, \tag{5.490}$$

which previously did not appear because of the second Dirac condition (5.411). It is the vacuum energy of two unphysical degrees of freedom for each momentum $\mathbf{k}$. This wrong vacuum energy may also be seen directly by bringing the Hamilton operator (5.413) to normal order using the commutation rule (5.391), yielding

$$H \;=\; \sum_{\mathbf{k}} k^0 \left(-a_{\mathbf{k}}^{\mu\dagger} a_{\mathbf{k},\mu} + \frac{1}{2} \right), \tag{5.491}$$

the second term showing the vacuum energy of *four* polarization degrees of freedom, rather than just the physical ones.

A heuristic remedy to the wrong vacuum energy in the Gupta-Bleuler formalism will be discussed below, to be followed by a more satisfatory one in Section 10.10.

Photon Propagator in Gupta Bleuler Approach

We now calculate the propagator of the A_μ-field in the Gupta-Bleuler quantization scheme, which is given by the expectation value in the pseudo-physical vacuum state

$$G^{\mu\nu}(x,x') = \langle 0_{\text{“phys”}} | T A^\mu(x) A^\nu(x') | 0_{\text{“phys”}} \rangle. \tag{5.492}$$

Expanding the vector field A^μ as in (5.404), and inserting it into (5.492), we obtain for $x_0 > x_0'$ the same contributions as in Eqs. (5.459)–(5.464), except that the expectation values are to be taken in the pseudo-physical vacuum state $|0_{\text{“phys”}}\rangle$, where only $a_{\mathbf{k},s}|0_{\text{“phys”}}\rangle = 0$ and $\langle 0_{\text{“phys”}}|a^\dagger_{\mathbf{k},s} = 0$. As a consequence, there are contibutions from the expectation values of the terms (5.461) yielding a polarization sum

$$\epsilon^{\mu *}(\mathbf{k},\bar{s})\epsilon^\nu(\mathbf{k},s) + \epsilon^{\mu *}(\mathbf{k},s)\epsilon^\nu(\mathbf{k},\bar{s}).$$

which, together with the transverse sum (5.465), adds up to

$$\sum_{\sigma=\pm 1} \epsilon^{\mu *}(\mathbf{k},\sigma)\epsilon^\nu(\mathbf{k},\sigma) - \epsilon^{\mu *}(\mathbf{k},s)\epsilon^\nu(\mathbf{k},\bar{s}) - \epsilon^{\mu *}(\mathbf{k},\bar{s})\epsilon^\nu(\mathbf{k},s) = -g^{\mu\nu}. \tag{5.493}$$

For $x_0 < x_0'$, the same expression is found with spacetime and Lorentz indices interchanged: $x \leftrightarrow x'$, $\mu \leftrightarrow \nu$, so that the propagator becomes

$$\begin{aligned} G^{\mu\nu}(x,x') &= \langle 0_{\text{``phys''}}|TA^\mu(x)A^\nu(x')|0_{\text{``phys''}}\rangle \\ &= -g^{\mu\nu}\left[\Theta(x_0-x_0')\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}e^{-ik(x-x')}+\Theta(x_0'-x_0)\frac{1}{V}\sum_{k}\frac{1}{2k^0}e^{ik(x-x')}\right] \end{aligned} \tag{5.494}$$

Up to the prefactor $-g^{\mu\nu}$ this agrees with Eq. (5.44) for the propagator $G(x,x')$ of the Klein-Gordon field for zero mass, which we write as in (5.59) as

$$\begin{aligned} G^{\mu\nu}(x,x') &= \langle 0|TA^\mu(x)A^\nu(x')|0\rangle \\ &= -g^{\mu\nu}\left[\Theta(x_0-x_0')G^{(+)}(x,x')+\Theta(x_0'-x_0)G^{(-)}(x,x')\right] \\ &= -g^{\mu\nu}G(x,x'). \end{aligned} \tag{5.495}$$

This photon propagator is much simpler than the previous one in (5.349), making it much easier to perform calculations, this being the main virtue of the Gupta-Bleuler quantization scheme. A second advantage of the propagator (5.495) is that in contrast to the noncovariant propagator (5.354), it is a proper Green function associated with the wave equation (5.374) in the $\alpha = 0$ -gauge, satifying the inhomogeneous field equation

$$-\partial^2 G^{\mu\nu}(x-x') = -g^{\mu\nu}i\delta^{(4)}(x-x'). \tag{5.496}$$

A further special feature of the Gupta-Bleuler quantization procedure which is worth pointing out is that the condition $a_{\mathbf{k},s}|\psi_{\text{``phys''}}\rangle = 0$, does not uniquely fix the pseudo-physical vacuum state $|0_{\text{``phys''}}\rangle$. The vacuum state $|0\rangle =$ is one possible choice, but infinitely many other states are equally good candidates, as long as their physical photon number are zero. Focusing attention only on states of a fixed photon momentum parallel to the z-axis, the zero-norm states (5.393) all satisfy the condition $a_{\mathbf{k},s}|\psi_{\text{``phys''}}\rangle = 0$. As a consequence, any superposition of such states

$$|\tilde{0}\rangle = |0\rangle + c_{\mathbf{k}}^{(1)}|0\rangle_1 + c_{\mathbf{k}}^{(2)}|0\rangle_2 + \dots \tag{5.497}$$

has a unit norm, contains no transverse photon, satisfies the condition $a_{\mathbf{k},s}|\tilde{0}\rangle = 0$, and is thus an equally good pseudo-vacuum state of the system.

The expectation value of the vector potential A^μ in this vacuum is nonzero. Its **k**th component is equal to the coefficient $c^{(1)}$ associated with this momentum, i.e., it is some function $c(\mathbf{k})$. Because of the second of the commutation rules (5.415), its **k**th Fourier component $\epsilon^\mu(\mathbf{k},\nu)a_{\mathbf{k},\nu}$ has an expectation $\epsilon^\mu(\mathbf{k},s)$, with a coefficient $c_{\mathbf{k}} = c_{\mathbf{k}}^{(1)}$:

$$\langle\tilde{0}|A^\mu|\tilde{0}\rangle = c_{\mathbf{k}}\epsilon^\mu(\mathbf{k},s), \tag{5.498}$$

i.e., it is proportional to the four-momentum k^μ. In x-space, the expectation value of such a field is equal to a pure gradient $\partial^\mu\Lambda(x)$ and carries no electromagnetic field.

The condition (5.487). implies that

$$\langle\tilde{0}|a^\dagger_{\mathbf{k},0}a_{\mathbf{k},0}|\tilde{0}\rangle = \langle\tilde{0}|a^\dagger_{\mathbf{k},3}a_{\mathbf{k},3}|\tilde{0}\rangle. \tag{5.499}$$

The two sides are equal to some function of $\mathbf{k}$, say ${k^0}^2\chi(\mathbf{k})$. In a covariant way, the vacuum is thus characterized by the expectations

$$\begin{aligned}\langle\tilde{0}|a^\dagger_{\mathbf{k},\nu}a_{\mathbf{k}',\nu'}|\tilde{0}\rangle &= k_\mu\epsilon^{\mu*}(\mathbf{k},\nu)k_\nu\epsilon^\nu(\mathbf{k},\nu')\chi(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'} \\ \langle\tilde{0}|a_{\mathbf{k},\nu}a^\dagger_{\mathbf{k}',\nu'}|\tilde{0}\rangle &= [-g^{\nu\nu'} + k_\mu\epsilon^{\mu*}(\mathbf{k},\nu)k_\nu\epsilon^\nu(\mathbf{k},\nu')\chi(\mathbf{k})]\delta_{\mathbf{k},\mathbf{k}'}.\end{aligned} \tag{5.500}$$

If we use any of these vacua and do not impose the condition (5.487), the propagator

$$G_{\tilde{0}}{}^{\mu\nu}(x-x') = \langle\tilde{0}|TA^\mu(x)A^\nu(x')|\tilde{0}\rangle \tag{5.501}$$

is a gauge-transformed version of the original one. Let us calculate it. Using (5.500) we have

$$\begin{aligned}G_{\tilde{0}}{}^{\mu\nu}(x-x') &= \langle\tilde{0}|TA^\mu(x)A^\nu(x')|\tilde{0}\rangle \\ &= \frac{1}{V}\sum_{\mathbf{k},\nu,\nu'}\frac{1}{2k^0}e^{-ik(x-x')}[-\Theta(x_0-x_0')g^{\nu\nu'} + k_{\mu'}\epsilon^{\mu'*}(\mathbf{k},\nu)k_{\nu'}\epsilon^{\nu'}(\mathbf{k},\nu')\chi(\mathbf{k})] \\ &\qquad\qquad\qquad\times\epsilon^{\mu*}(\mathbf{k},\nu)\epsilon^\nu(\mathbf{k},\nu') \\ &= \frac{1}{V}\sum_{\mathbf{k},\nu,\nu'}\frac{1}{2k^0}e^{ik(x-x')}\ [-\Theta(x_0'-x_0)g^{\nu\nu'} + k_{\mu'}\epsilon^{\mu'*}(\mathbf{k},\nu)k_{\nu'}\epsilon^{\nu'}(\mathbf{k},\nu')\chi(\mathbf{k})] \\ &\qquad\qquad\qquad\times\epsilon^{\mu*}(\mathbf{k},\nu)\epsilon^\nu(\mathbf{k},\nu') \\ &= \frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}e^{-ik(x-x')}[-\Theta(x_0-x_0')g^{\mu\nu} + k^\mu k^\nu\chi(\mathbf{k})] \\ &\quad+\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}e^{ik(x-x')}\ [-\Theta(x_0'-x_0)g^{\mu\nu} + k^\mu k^\nu\chi(\mathbf{k})].\end{aligned} \tag{5.502}$$

The $g^{\mu\nu}$-terms are again equal to $G^{\mu\nu}$ of Eq. (5.495). The $k^\mu k^\nu$ terms may be placed outside the integrals where they become spacetime derivatives $-\partial^\mu\partial^\nu$ of a function

$$F(x-x') = \frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2k^0}[e^{-ik(x-x')} + e^{ik(x-x')}]\chi(\mathbf{k}). \tag{5.503}$$

Thus we find

$$G_{\tilde{0}}{}^{\mu\nu}(x-x') = G_0{}^{\mu\nu}(x-x') - \partial^\mu\partial^\nu F(x-x'). \tag{5.504}$$

Physical observables must, of course, be independent of $F(x-x')$. This will be proved in Chapter 10 after Eq. (10.92).

Note that in contrast to $G^{\mu\nu}(x-x')$, the Fourier components of $F(x-x')$ are restricted to the light cone. This is seen more explicitly by rewriting the sums in (5.503) as integrals, and introducing the δ-function

$$\delta(k^2) = \frac{1}{2\omega_{\mathbf{k}}}[\delta(k^0-\omega_{\mathbf{k}}) + \delta(k^0+\omega_{\mathbf{k}})], \tag{5.505}$$

so that $F(x-x')$ is equal to the four-dimensional integral

$$F(x-x') = \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-x')} 2\pi\delta(k^2)\chi(\mathbf{k}). \tag{5.506}$$

The function $F(x-x')$ is therefore a solution of the Klein-Gordon equation $\partial^2 F(x-x') = 0$. This is the same type of freedom we are used to from Green functions. Different Green functions satisfying the same inhomogeneous differential equation

$$-\partial^2 G^{\mu\nu} = -ig^{\mu\nu}\delta^{(4)}(x-x'). \tag{5.507}$$

differ from each other by solutions of the homogeneous differential equation, and so do the propagators $G_{\bar{0}}{}^{\mu\nu}(x-x')$ and $G_0{}^{\mu\nu}(x-x')$ coming from different vacuum states.

Remedy to Wrong Vacuum Energy in Gupta-Bleuler Approach

In the Hamilton operators (5.489) and (5.491) we found an important failure of the Gupta-Bleuler quantization scheme. The energy contains also the vacuum oscillations of the two unphysical degrees of freedom oscillating in 0- and the **k**-direction. Due to the opposite commutation rules of the associated creation and annihilation operators, there is no cancellation of the two contributions. The Gupta-Bleuler approach eliminates the unphysical modes from all multiparticle states except for the vacuum. The elimination of this vacuum energy in the covariant approach was achieved only much later by Fadeev and Popov.[23] Their method was developed in the attempt to quantizing nonabelian gauge theories. There the elimination of the unphysical gauge degrees of freedom can no longer be done with the help of the Gupta-Bleuler subsidiary condition (5.487). Essential to their approach is the use of the functional integral formulation of quantum field theory. In it, all operator calculations are replaced by products of infinitely many integrals over classical fluctuating fields. This formulation will be introduced in Chapter 10. When fixing a covariant gauge in the gauge-invariant quantum partition function of the electromagnetic fields, one must multiply the functional integral by a factor removing the partition function of the unphysical modes. At zero temperature, this factor subtracts, in the abelian gauge theory of QED, precisely the vacuum energies of the two unphysical modes. The removal requires an equal amount of negative vacuum energy. In Eq. (5.232) we have observed that fermions have negative vacuum energies. The subtraction of the unphysical vaccum energies can therefore be achieved by introducing two fictitious Fermi fields, a ghost field $C(x)$ and anti-ghost field $\bar{C}(x)$. They are completely unphysical objects with spin zero. They never appear in the physical Hilbert space,[24] i.e., the physical state vectors satisfy the conditions

$$C^\dagger(x)|0_{\rm phys}\rangle = 0, \qquad \bar{C}^\dagger(x)|0_{\rm phys}\rangle = 0. \tag{5.508}$$

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[23] L.D. Fadeev and V.N. Popov, Phys. Lett. B *25*, 29 (1967).

[24] For this reason, the wrong spin-statistics connection to be derived in Section 4.6 does not cause causality problems.

These fields are called *Fadeev-Popov ghosts*. In QED with gauge $\partial_\mu A^\mu(x) = 0$, their *only* contribution lies in the negative vacuum energy

$$E_0^{\text{ghosts}} = -2\sum_{\mathbf{k}} \frac{k^0}{2} \tag{5.509}$$

which cancels the excessive vacuum energy (5.490) in the Gupta-Bleuler approach.

In quantum electrodynamics, the effect of the ghosts is trivial so that their introduction is superfluous for all purposes except for calculating the vacuum energy. This is the reason why their role was recognized only late in the development.[25]

In nonabelian gauge theories, the ghost fields have nontrivial interactions with the physical particles, which must be included in all calculations to make the theory consistent.

In the light of this development, the correct way of writing the Lagrangian density of the free-photon field is

$$\mathcal{L}_{\text{tot}} = \mathcal{L} + \mathcal{L}_{\text{GF}} + \mathcal{L}_{\text{ghost}} = -\frac{1}{4}{F_{\mu\nu}}^2 - D(x)\partial^\mu A_\mu(x) + \alpha D^2(x)/2 - i\partial_\mu \bar{C}\partial^\mu C. \tag{5.510}$$

We shall see that this Lagrangian has an interesting new global symmetry between the Bose fields A^μ, D and the Fermi fields $C, \bar{C}$, called supersymmetry, which will be discussed in Chapter 23. In this context it is called BRS symmetry.[26]

The Gupta-Bleuler gauge condition plus the subsidiary ghost conditions (5.508) eliminating the unphysical degrees of freedom are equivalent to requiring that the charges generating all global symmetry transformations annihilate the physical vacuum. Although structurally somewhat complicated, this is the most satisfactory way of formulating the covariant quantization procedure of the photon field.

The pseudophysical vacuum $|0_{\text{phys}'}\rangle$ of the Gupta-Bleuler approach has a unit norm, which is an important advantage over the physical vacuum $|0_{\text{phys}'}\rangle$ of the Dirac approach. In axiomatic quantum field theory it can be proved[27] that for any local operator $\mathcal{O}(x)$

$$\mathcal{O}(x)|0\rangle = 0 \quad \text{if and only if} \quad \mathcal{O}(x) = 0. \tag{5.511}$$

This is the reason why the Gupta-Bleuler subsidiary condition involves necessarily a nonlocal operator. Recall that the operator in (5.487) involves only the positive-frequency part of the local field $D(x)$. The negative frequencies would be needed to make the field local. This will become clear in proving the spin-statistic relation in Section 5.8.

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[25] R.P. Feynman, Acta Phys. Polonica, *24*, 697 (1963).

[26] C. Becchi, A. Rouet, and R. Stora, Ann. Phys. *98*, 287 (1976).

[27] R.F. Streater and A.S. Wightman, *PCT, Spin & Statistics, and All That*, Benjamin, New York, 1964, pp. 139, 163; F. Strocchi, Phys. Rev. *162*, 1429 (1967). See also the discussion of N. Nakanishi, in *Quantum Electrodynamics*, ed. by T. Kinoshita, World Scientific, Singapore, 1990, pp. 36–80 .

Arbitrary Gauge Parameter α

A quantization of the electromagnetic field is possible also for different values of the gauge parameter α in the Lagrangian density (5.362) which so far has been set equal to unity, for simplicity. For an arbitrary value of α, the field equation (5.366) can be written as

$$L_{\mu\nu}(i\partial)A^{\nu}(x)=0, \tag{5.512}$$

with the differential operator

$$L_{\mu\nu}(i\partial)\equiv-\partial^2 g_{\mu\nu}+\left(1-\frac{1}{\alpha}\right)\partial_\mu\partial_\nu. \tag{5.513}$$

Multiplying Eq. (5.512) by ∂^μ we find that the vector potential cannot have any four-divergence:

$$\partial_\mu A^\mu(x)=0. \tag{5.514}$$

In a gauge-invariant formulation, this property can be chosen as the *Lorentz gauge conditon*. Since the Lagrangian density (5.362) breaks gauge invariance, the Lorentz condition is a consequence of the equations of motion. For a field $A^\mu(x)$ satisfying the Lorentz gauge condition, the equations of motion reduce to 4 Klein-Gordon equations, just as before in the Feynman case $\alpha=1$ [see (5.374)]:

$$-\partial^2 A^\mu(x)=0. \tag{5.515}$$

We shall not go through the entire quantization procedure and the derivation of the propagator in this case. What can be given without much work is the Green function defined by the inhomogeneous field equation

$$L_{\mu\nu}(i\partial)G^{\nu\kappa}(x-x')=-i\delta_\mu{}^\kappa\delta^{(4)}(x-x'). \tag{5.516}$$

In momentum space, it reads

$$L_{\mu\nu}(k)G^{\nu\kappa}(k)=-i\delta_\mu{}^\kappa. \tag{5.517}$$

with the 4×4 -matrix

$$L_{\mu\nu}(k)=k^2\left(g_{\mu\nu}-\frac{k_\mu k_\nu}{k^2}\right)+\frac{k^2}{\alpha}\frac{k_\mu k_\nu}{k^2}. \tag{5.518}$$

This matrix has an eigenvector k^μ with an eigenvalue k^2/α, and three eigenvectors orthogonal to it with eigenvalues k^2. associated with the eigen For a finite α, the matrix has an inverse, which is found by rewriting $L_{\mu\nu}(k)$ as

$$L^{\mu\nu}(k)=k^2P_{T\,\mu\nu}(k)+\frac{k^2}{\alpha}P_{L\,\mu\nu}(k). \tag{5.519}$$

with

$$\begin{aligned} P_T^{\mu\nu}(k) &= g^{\mu\nu}-\frac{k^\mu k^\nu}{k^2}, \\ P_L^{\mu\nu}(k) &= \frac{k^\mu k^\nu}{k^2}. \end{aligned} \tag{5.520}$$

These matrices are projections, since both satisfy the defining relation

$$P^{\mu\nu}P_{\nu}{}^{\kappa} = P^{\mu\kappa}. \tag{5.521}$$

The inverse of (5.519) is found by inverting the coefficients in front of $P_T(k)$ and $P_L(k)$:

$$L^{-1\mu\nu}(k) = \frac{1}{k^2}P_T^{\mu\nu}(k) + \frac{\alpha}{k^2}P_L^{\mu\nu}(k) = \frac{1}{k^2}\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2}\right) + \frac{\alpha}{k^2}\frac{k^\mu k^\nu}{k^2}, \tag{5.522}$$

so that we can solve (5.517) by

$$G^{\mu\nu}(k) = -iL^{-1\mu\nu}(k). \tag{5.523}$$

The propagator has therefore the Fourier representation

$$G^{\mu\nu}(x-x') = \int \frac{d^4k}{(2\pi)^4}e^{-ik(x-x')}\frac{i}{k^2+i\eta}\left[-g^{\mu\nu} + (1-\alpha)\frac{k^\mu k^\nu}{k^2+i\eta}\right]. \tag{5.524}$$

As usual, we have inserted imaginary parts $i\eta$ to regularize the integral in the same way as in the peopagator of the scalar field. For the term $k^\mu k^\nu/(k^2+i\eta)$ the prescription how to place the additional poles is not immediately obvious. The best way to derive it is by giving the photon a small mass and setting it later equal to zero. The reader is referred to the next section where the massive vector meson is treated. The reader may be worried about the physical meaning of the double-pole in the integrand of the propagator (5.524). A pole in the propagator is associated with a particle state in the Hilbert space. How does a double pole manifest itself in the Hilbert space? Heisenberg called the associated state a *dipole ghost*.[28] Instead of satisfying a Schrödinger equation

$$(E-H)|\psi\rangle = 0, \tag{5.525}$$

such a state satisfies the two equations

$$(E-H)|\psi\rangle \neq 0, \qquad (E-H)^2|\psi\rangle = 0, \tag{5.526}$$

and is unphysical. In the present context. these unphysical states do not cause any problems since they are an artifact of the gauge fixing and do not contribute to any observable quantity, due to gauge invariance. The same will be true in the presence of moving charges in Chapter 10.

It is possible to derive the same result for the propagator of the photon field governed by the general Lagarangian density (5.361). This exercise is left to the reader.

Since the $D(x)$-field is now equal to $\partial_\mu A^\mu(x)/\alpha$ [recall (5.364)], the gauge parameter α enters in various commutation rules between $A^\mu(\mathbf{x},t)$ and $\dot{A}^\mu(\mathbf{x},t)$. Proceeding as in Eqs. (5.380)–(5.388), we find that the gauge parameter α enters into the commutation rules among $A^\mu(\mathbf{x},t)$ and $\dot{A}^\mu(\mathbf{x},t)$ in Eqs. (5.384) and (5.387) as follows:

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[28] W. Heisenberg, Nucl. Phys. *4*, 532 (1957).

$$\begin{aligned}
[\dot{A}^0(\mathbf{x},t), A^0(\mathbf{x}',t)] &= \alpha[D(\mathbf{x},t), A^0(\mathbf{x}',t)] = \alpha i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), && (5.527)\\
\left[\dot{A}^i(\mathbf{x},t), \dot{A}^j(\mathbf{x}',t)\right] &= 0, && (5.528)\\
\left[\dot{A}^0(\mathbf{x},t), \dot{A}^i(\mathbf{x}',t)\right] &= -(1-\alpha)i\partial_i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), && (5.529)\\
\left[\dot{A}^0(\mathbf{x},t), \dot{A}^0(\mathbf{x}',t)\right] &= 0. && (5.530)
\end{aligned}$$

The other commutators (5.382), (5.385), and (5.386) remain unchanged.

These commutators are needed to verify that the vacuum expectation of the time-ordered product

$$G^{\mu\nu}(x-x') \equiv \langle 0|TA^\mu(x)A^\nu(x')|0\rangle \qquad (5.531)$$

satisfies the field equation with a δ-function source (5.632). The proof of this is nontrivial:

$$\begin{aligned}
&-\left[\partial^2 g_{\mu\nu} - \left(1-\frac{1}{\alpha}\right)\partial_\mu\partial_\nu\right]G^{\nu\kappa}(x-x') = \\
&-\langle 0|T\left[\partial^2 g_{\mu\nu} - \left(1-\frac{1}{\alpha}\right)\partial_\mu\partial_\nu\right]A^\nu(x)A^\kappa(x')|0\rangle - \delta(x^0-x'^0)g_{\mu\nu}\langle 0|[\dot{A}^\nu(x), A^\kappa(x')]|0\rangle \\
&+\left(1-\frac{1}{\alpha}\right)g_{0\mu}\delta(x^0-x'^0)\langle 0|[\partial_\nu A^\nu(x), A^\kappa(x')]|0\rangle = -i\delta_\mu{}^\kappa\delta^{(4)}(x-x'), \qquad (5.532)
\end{aligned}$$

the right-hand requiring the commutation relations (5.527)–(5.530).

It is useful to check the consistency of the propagator with the canonical commutation rules. This is done in Appendix 5B.

5.4.3 Behavior under Discrete Symmetries

Under P,C,T, the vector potential has the transformation properties [recall Section 3.6]:

$$\begin{aligned}
A^\mu(x) &\xrightarrow{P} A'^\mu_P(x) = \tilde{A}^\mu(\tilde{x}), && (5.533)\\
A^\mu(x) &\xrightarrow{T} A'^\mu_T(x) = \tilde{A}^\mu(x_T), && (5.534)\\
A^\mu(x) &\xrightarrow{C} A'^\mu_C(x) = -A^\mu(x). && (5.535)
\end{aligned}$$

The photon has a negative charge parity which coincides with that of the vector current $V^\mu(x) = \bar{\psi}(x)\gamma^\mu\psi(x)$ formed from two Dirac fields in Table 3.1, to which it will later be coupled in Chapter 10.

These properties are implemented in the second-quantized Hilbert space by transforming the photon creation operators as follows:

$$\begin{aligned}
\mathcal{P}a^\dagger_{\mathbf{k},\nu}\mathcal{P}^{-1} &\equiv a^\dagger_{-\mathbf{k},-\nu}, && (5.536)\\
\mathcal{T}a^\dagger_{\mathbf{k},\nu}\mathcal{T}^{-1} &\equiv a^\dagger_{-\mathbf{k},\nu}, && (5.537)\\
\mathcal{C}a^\dagger_{\mathbf{k},\nu}\mathcal{C}^{-1} &\equiv -a^\dagger_{\mathbf{k},\nu}. && (5.538)
\end{aligned}$$

The annihilation operators transform by the hermitian-adjoint relations.

5.5 MASSIVE VECTOR BOSON

Besides the photon, there exist also massive vector bosons. The most important examples are the fundamental vector bosons mediating the weak interactions, as we shall see in Chapter 24. They can be electrically neutral or carry an electric charge $\pm e$. There exist also strongly interacting vector particles of a composite nature. They are short-lived and only observable as resonances in scattering experiments, the most prominent being a resonance in the two-pion scattering amplitude. These are the famous ρ-mesons which will be discussed in Chapter 22. They also carry charges $0, \pm 1$. The actions of a neutral and charged massive vector field $V^\mu(x)$ were given in Eqs. (3.319) and (3.321):

$$\mathcal{A} = \int d^4x \, \mathcal{L}(x) = \int d^4x \left(-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} M^2 V_\mu V^\mu \right), \tag{5.539}$$

and

$$\mathcal{A} = \int d^4x \, \mathcal{L}(x) = \int d^4x \left(-\frac{1}{2} F^*_{\mu\nu} F^{\mu\nu} + M^2 V^*_\mu V^\mu \right), \tag{5.540}$$

with the equations of motion

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu = 0, \tag{5.541}$$

or

$$[(-\partial^2 - M^2) g_{\mu\nu} + \partial_\mu \partial_\nu] V^\mu(x) = 0. \tag{5.542}$$

implying that the vector field $V^\mu(x)$ has no four-divergence:

$$\partial_\mu V^\mu(x) = 0, \tag{5.543}$$

and the Klein-Gordon equations

$$(-\partial^2 - M^2) V^\mu(x) = 0. \tag{5.544}$$

It will sometimes be convenient to view the photon as an $M \to 0$ -limit of a massive vector meson. In this case we have to add a gauge fixing term to the Lagangian to have a proper limit. Thus we consider the Lagrangian

$$\mathcal{A} = \int d^4x \, \mathcal{L}(x) = \int d^4x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} M^2 V_\mu V^\mu - \frac{1}{2\alpha} \left(\partial_\mu V^\mu \right)^2 \right\}, \tag{5.545}$$

leading to a field equation

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu + \frac{1}{\alpha} \partial^\nu \partial_\mu V^\mu = 0, \tag{5.546}$$

or

$$\left[(-\partial^2 - M^2) g_{\mu\nu} + \left(1 - \frac{1}{\alpha} \right) \partial_\mu \partial_\nu \right] V^\mu(x) = 0. \tag{5.547}$$

Multiplying (5.545) with ∂_ν from the left gives for the divergence $\partial_\nu V^\nu$ the Klein-Gordon equation

$$(\partial^2 + \alpha M^2) \partial_\nu V^\nu(x) = 0, \tag{5.548}$$

which yields the constraint (5.543) in the limit $\alpha \to \infty$.

5.5.1 Field Quantization

The canonical field momenta are

$$\pi_\mu = \frac{\partial \mathcal{L}}{\partial[\partial_0 V^\mu]} = -F^*_{0\mu}, \tag{5.549}$$

where the complex conjugation is of course irrelevant for a real field. As for electromagnetic fields, the zeroth component $V^0(x)$ has no canonical field momentum. There is again a primary constraint $\pi_0 = 0$. This is of course due to the fact the Euler-Lagrange equation Eq. (3.324) for $V^0(x)$ is not a dynamical field equation.

For the spatial components $V^i(x)$, the nonvanishing canonical equal-time commutation rules are

$$\begin{aligned} [\pi_i(\mathbf{x},t), V^j(\mathbf{x}',t)] &= -i\delta_i{}^j\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \\ [\pi_i^\dagger(\mathbf{x},t), V^{j\dagger}(\mathbf{x}',t)] &= -i\delta_i{}^j\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \end{aligned} \tag{5.550}$$

The commutators involving $V^0(\mathbf{x},t)$ can be calculated from this using relation (3.324), yielding

$$[V^{0\dagger}(\mathbf{x},t), V^i(\mathbf{x}',t)] = \frac{i}{M^2}\partial_i\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{5.551}$$

and

$$[V^0(\mathbf{x},t), V^i(\mathbf{x}',t)] = 0. \tag{5.552}$$

To exhibit the particle content in the second-quantized fields, we now expand $V^\mu(x)$ into the complete set of classical solutions of Eqs. (5.541) and (5.543) in a large but finite volume V:

$$V^\mu(x) = \sum_{\mathbf{k},s_3=0,\pm1} \frac{1}{\sqrt{2Vk^0}}\left[e^{-ikx}\epsilon^\mu(\mathbf{k},s_3)a_{\mathbf{k},s_3} + e^{ikx}\epsilon^{\mu*}(\mathbf{k},s_3)b^\dagger_{\mathbf{k},s_3}\right]. \tag{5.553}$$

For real vector fields, the same expansions hold with particles and antiparticles identified.

Dealing with massive vector particles, we may choose to label the polarization states by canonical spin orientations s_3, the third components of angular momentum in the particle's rest frame. The polarization vectors were given explicitly in Eq. (3.328).

As for scalar and Dirac fields, we have associated the expansion coefficients of the plane waves of negative energy e^{ikx} with a creation operator $b^\dagger_{\mathbf{k},s_3}$ rather than a second type of annihilation operator $d_{\mathbf{k},s_3}$. In principle, the polarization vector associated with the antiparticles could have been some charge-conjugate polarization vector $\epsilon^\mu_c(\mathbf{k},s_3)$ in analogy to the spinors $v(\mathbf{p},s_3) = u^c(\mathbf{p},s_3)$ [recall (3.617)]. For a vector field , however, which transforms under real 4×4 Lorentz matrices $\Lambda^\mu{}_\nu$, charge conjugation changes the polarization vector (or tensor) simply into the complex conjugate one. This will be proved below.

Alternatively we may expand the field $V^\mu(x)$ in terms of helicity polarization states as

$$V^\mu(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2Vk^0}} \sum_{\lambda=\pm1,0} \left[e^{-ipx}\epsilon_H^\mu(\mathbf{k},\lambda)a_{\mathbf{k},\lambda} + e^{ipx}\epsilon_H^{\mu*}(\mathbf{k},\lambda)b^\dagger_{\mathbf{k},\lambda}\right]. \qquad (5.554)$$

where $\epsilon_H^\mu(\mathbf{k},\lambda)$ are the polarization vectors (3.335).

The quantization of the massive vector field with the Lagrangian (5.545) proceeds most conveniently by introducing a transverse field

$$V_\mu^T(x) \equiv V_\mu + \frac{1}{\alpha M^2}\partial_\mu\partial_\nu V^\nu(x), \qquad (5.555)$$

which is divergenceless as a consequence of 5.548:

$$\partial^\mu V_\mu^T(x) = 0. \qquad (5.556)$$

The full vector field is then a sum of a purely transverse and the gradient of a scalar field $\partial_\nu V^\nu(x)$:

$$V_\mu(x) = V_\mu^T(x) - \frac{1}{\alpha M^2}\partial_\mu\partial_\nu V^\nu(x). \qquad (5.557)$$

It can be expanded in terms of three cration and annihilation operators $a^\dagger_{\mathbf{k},\lambda}$, $a_{\mathbf{k},\lambda}$ for the three physical polarization states with helicites $\lambda = 0, \pm1$, and an extra pair of operators $a^\dagger_{\mathbf{k},s}$, $a_{\mathbf{k},s}$ for the scalar degree of freedom. The commutation rules are

$$\begin{aligned} [a_{\mathbf{k},\nu}, a_{\mathbf{k}',\nu'}] &= [a^\dagger_{\mathbf{k},\nu}, a^\dagger_{\mathbf{k}',\nu'}] = 0, \\ [a_{\mathbf{k},\nu}, a^\dagger_{\mathbf{k}',\nu'}] &= -\delta_{\mathbf{k},\mathbf{k}'}g_{\nu\nu'}. \end{aligned} \qquad (5.558)$$

where ν runs through $\lambda = 0, \pm1$ and s and the diagonal metric $g_{\nu\nu'}$ has a negative signature for $\lambda = 0, \pm1$ and a positive one for $\nu = s$. These commutation rules have the same form as those in (5.389), except for the different meaning of the labels ν. The properly quantized field is then

$$\begin{aligned} V^\mu(x) &= \sum_{\mathbf{k},\lambda=0,\pm1} \frac{1}{\sqrt{2Vk^0}}\left[e^{-ikx}\epsilon^\mu(\mathbf{k},\lambda)a_{\mathbf{k},\lambda} + \epsilon^{\mu\,*}(\mathbf{k},\lambda)a^\dagger_{\mathbf{k},\lambda}\right] \\ &\quad + \frac{k^\mu}{M}\frac{1}{\sqrt{2Vk^0}}\left[e^{-ikx}\epsilon^\mu(\mathbf{k},s)a_{\mathbf{k},s} + \epsilon^{\mu\,*}(\mathbf{k},s)a^\dagger_{\mathbf{k},s}\right]. \end{aligned} \qquad (5.559)$$

5.5.2 Energy of Massive Vector Particle

The energy can be calculated in close analogy with that of photons. We shall consider a real field, and admit an additional coupling to an external current density $j^\mu(x)$ to the system, with an interaction

$$\mathcal{L}_{\text{int}} = -j^\mu(x)V_\mu(x). \qquad (5.560)$$

This causes only a minor additional labor but will be useful to understand a special feature of the massive propagator to be calculated in the next section. The current term changes the equations of motion (5.541) to

$$\partial_\mu F^{\mu\nu} + M^2 V^\nu - j^\nu = 0, \tag{5.561}$$

implying for the non-dynamical zeroth component of $V^\mu(x)$ the relation

$$V^0(x) = \frac{1}{M^2}\left[\boldsymbol{\nabla}\cdot\dot{\mathbf{V}}(x) + \boldsymbol{\nabla}^2 V^0(x) - j^0(x)\right]. \tag{5.562}$$

rather than (3.324). As in electromagnetism, we rename the negative of the canonical field momenta (5.549) the "electric" field strength of the massive vector field:

$$\mathbf{E}(x) \equiv -\boldsymbol{\pi}(x) = -\dot{\mathbf{V}}(x) - \boldsymbol{\nabla}V^0(x). \tag{5.563}$$

Combining this with (5.562), we obtain

$$\dot{\mathbf{V}}(x) = -\mathbf{E}(x) - \boldsymbol{\nabla}V^0(x) = -\mathbf{E}(x) + \frac{1}{M^2}\boldsymbol{\nabla}[\boldsymbol{\nabla}\cdot\mathbf{E}(x) - j^0(x)]. \tag{5.564}$$

We now form the Hamiltonian density (5.328) as the Legendre transform

$$\mathcal{H} = \sum_{i=1}^{3}\pi_i\dot{V}^i - \mathcal{L} - \mathcal{L}_{\rm int}. \tag{5.565}$$

Inserting (5.564) we obtain

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int}, \tag{5.566}$$

with a free Hamiltonian density

$$\mathcal{H} = \frac{1}{2}\left[\mathbf{E}^2 + \mathbf{B}^2 + \frac{1}{M^2}\left(\boldsymbol{\nabla}\cdot\mathbf{E}\right) + M^2\mathbf{V}^{\mathbf{2}}\right], \tag{5.567}$$

and an interacting one

$$\mathcal{H}_{\rm int} = \mathbf{j}\cdot\mathbf{V} - \frac{1}{M^2}j^0\boldsymbol{\nabla}\cdot\mathbf{E} + \frac{1}{M^2}j^{0^2}. \tag{5.568}$$

We have introduced

$$\mathbf{B}(x) = \boldsymbol{\nabla}\times\mathbf{V}(x) \tag{5.569}$$

in analogy with the magnetic field of electromagnetism [compare (5.328)]

Discarding again the external current, we form the free Hamiltonian $H_0 = \int d^3x\,\mathcal{H}_0$, express $\mathbf{E}(x)$ as $-\dot{\mathbf{V}} - \boldsymbol{\nabla}V^0$, and $\boldsymbol{\nabla}\cdot\mathbf{E}$ as $-M^2V^0$, and find the Hamiltonian

$$H = \int d^3x\,\left\{\frac{1}{2}\left[-\dot{V}^\mu\dot{V}^\mu - \boldsymbol{\nabla}V^\mu\cdot\boldsymbol{\nabla}V_\mu - M^2V^\mu V_\mu\right] - \boldsymbol{\nabla}\cdot(\mathbf{E}\,V^0)\right\}. \tag{5.570}$$

The last term is a surface term that can be omitted in an infinite volume. Inserting the expansion (5.554) for the field operator, and proceeding as in the case of the photon energy (5.344), we obtain the energy

$$H = \sum_{k,\lambda=0,\pm1} k^0 \left(a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + \tfrac{1}{2}\right). \tag{5.571}$$

This contains a vacuum energy

$$E_0 \equiv \langle 0|H|0\rangle = \frac{1}{2} \sum_{\mathbf{k},\lambda=0\pm1} k^0 = \frac{3}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}}, \tag{5.572}$$

due to the zero-point oscillations, the factor 3 counting the different polarization states.

5.5.3 Propagator of Massive Vector Particle

Let us now calculate the propagator of the massive vector particle from the vacuum expectation value of the time-ordered product of two vector fields. As in (5.348) we find

$$\begin{aligned} G^{\mu\nu}(x,x') &= \Theta(x_0 - x_0')\frac{1}{2V}\sum_{\mathbf{k}} \frac{1}{k^0} e^{-ik(x-x')} \sum_{\lambda} \epsilon^{\mu}(\mathbf{k},\lambda)\epsilon^{\nu *}(\mathbf{k},\lambda) \\ &+ \Theta(x_0' - x_0)\frac{1}{2V}\sum_{\mathbf{k}} \frac{1}{k^0} e^{ik(x-x')} \sum_{\lambda} \epsilon^{\nu}(\mathbf{k},\lambda)\epsilon^{\mu *}(\mathbf{k},\lambda). \end{aligned} \tag{5.573}$$

and insert the completeness relation (3.333) to write

$$\begin{aligned} G^{\mu\nu}(x,x') &= \Theta(x_0 - x_0')\frac{1}{2V}\sum_{\mathbf{k}} \frac{1}{k^0} e^{-ik(x-x')} \left(-g^{\mu\nu} + \frac{k^\mu k^\nu}{M^2}\right) \\ &+ \Theta(x_0' - x_0)\frac{1}{2V}\sum_{\mathbf{k}} \frac{1}{k^0} e^{ik(x-x')} \left(-g^{\mu\nu} + \frac{k^\mu k^\nu}{M^2}\right). \end{aligned} \tag{5.574}$$

This expression has precisely the general form (5.270) with the polarization sums of particles and antiparticles being equal to one another. The common polarization sum can be pulled in front of the Heaviside functions yielding

$$\begin{aligned} &G^{\mu\nu}(x,x') \\ &= \left(-g^{\mu\nu} - \frac{\partial^\mu\partial^\nu}{M^2}\right)\left[\Theta(x_0 - x_0')G^{(+)}(x-x') + \Theta(x_0' - x_0)G^{(-)}(x-x')\right] \\ &+\frac{1}{M^2}\{[\partial^\mu\partial^\nu, \Theta(x^0 - x'^0)]G^{(+)}(x-x') + [\partial^\mu\partial^\nu, \Theta(x'^0 - x^0)]G^{(-)}(x-x')\}. \end{aligned} \tag{5.575}$$

The bracket in the first expression is equal to the Feynman propagator of the scalar field. The second term can only contribute for $\mu,\nu = 0,0$. For $\mu = i$ and $\nu = j$, it vanishes trivially. For $\mu = 0$ and $\nu = i$, it gives

$$\frac{1}{M^2}[\partial^i\delta(x^0 - x'^0)G^{(+)}(x-x')\partial^i\delta(x'^0 - x^0)G^{(-)}(x-x')].$$

Since

$$\delta(x^0 - x'^0)G^{(+)}(x - x') = \delta(x'^0 - x^0)G^{(-)}(x - x'),$$

this vanishes. For $\mu = \nu = 0$, on the other hand, we write

$$\begin{aligned}[\partial_0\partial_0, \Theta(x^0 - x'^0)] &= \partial_0\delta'(x^0 - x'^0) + 2\delta(x^0 - x'^0)\partial_0, \\ [\partial_0\partial_0, \Theta(x'^0 - x^0)] &= -\partial_0\delta(x'^0 - x^0) - 2\delta(x^0 - x'^0)\partial_0,\end{aligned}$$

and

$$\partial_0 G^{(\pm)}(\mathbf{x} - \mathbf{x}') = \mp\frac{i}{2}\delta^{(3)}(\mathbf{x} - \mathbf{x}') \tag{5.576}$$

to obtain from the last terms $-2i\delta^{(4)}(x - x')$. By a calculation like (5.41) we see that the first terms remove from this the factor 2. Thus we find for the Feynman propagator of the massive vector field

$$\begin{aligned}G^{\mu\nu}(x, x') &= -\int\frac{d^4k}{(2\pi)^4}e^{-ik(x-x')}\frac{i}{k^2 - M^2 + i\eta}\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2}\right) \\ &\quad -\frac{i}{M^2}\delta_{\mu 0}\delta_{\nu 0}\delta^{(4)}(x - x').\end{aligned} \tag{5.577}$$

Only the first term is a Lorentz tensor. The second term destroys the covariance and is called a *Schwinger term*. Let us trace its origin in momentum space. If we replace the Heaviside functions in (5.573) by the Fourier integrals (5.60), we find for the propagator a representation of the type (5.277):

$$G^{\mu\nu}(x - x') = \int\frac{d^4k}{(2\pi)^4}\frac{i}{2\omega_{\mathbf{p}}}\left[\frac{P^{\mu\nu}(\omega_{\mathbf{k}}, \mathbf{k})}{k^0 - \omega_{\mathbf{k}} + i\eta} - \frac{P^{\mu\nu}(-\omega_{\mathbf{k}}, \mathbf{k})}{k^0 + \omega_{\mathbf{k}} - i\eta}\right]e^{-ip(x-x')}, \tag{5.578}$$

with

$$P^{\mu\nu}(\omega_{\mathbf{k}}, k) \equiv P^{\mu\nu}(k^0, k)\Big|_{k^0=\omega_{\mathbf{k}}} \equiv -\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2}\right)\Bigg|_{k^0=\omega_{\mathbf{k}}}. \tag{5.579}$$

Expression (5.578) is a tensor only if the on-shell energy ω in the argument of $P(k)$ is replaced by the off-shell integration variable k^0. The difference between (5.579) and such a covariant version has two contributions: one from the linear term in k^0, and one from the quadratic term. The first vanishes by the same mechanism as in the Dirac discussion of (5.277). The quadratic term contributes only for $(\mu, \nu) = (0, 0)$, where

$$P^{00}(\omega_{\mathbf{k}}, \mathbf{k}) - P^{00}(k) = \frac{\omega_{\mathbf{k}}^2 - k^{02}}{M^2}. \tag{5.580}$$

The combination $\omega_{\mathbf{k}}^2 - k^{02} = M^2 - k^2$ cancels the denominators in (5.578), thus producing precisely the δ-function term (5.577).

The covariant part of the propagator coincides with the Green function of the field equation (5.542). Indeed, the differential operator on the left-hand side can be written in analogy with (5.519), as

$$L_{\mu\nu}(i\partial)G^{\nu\kappa}(x-x') = -i\delta_{\mu}{}^{\kappa}\delta^{(4)}(x-x'), \tag{5.581}$$

so that the calculation of the Green function requires inverting the matrix in momentum space [the analog of (5.519)]

$$L_{\mu\nu}(k) = (k^2 - M^2)P_{T\,\mu\nu}(k) - M^2 P_{L\,\mu\nu}(k). \tag{5.582}$$

This has inverse

$$L^{-1\,\mu\nu}(k) = \frac{1}{k^2-M^2}P_T^{\mu\nu}(k) - \frac{1}{M^2}P_L^{\mu\nu}(k) = \frac{1}{k^2-M^2}\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{M^2}\right), \tag{5.583}$$

yielding the solution of (5.581) in momentum space:

$$G^{\mu\nu}(k) = -iL^{-1\,\mu\nu}(k). \tag{5.584}$$

This is precisely the Fourier content in the first term of (5.577). The mass contains an infinitesimal $-i\eta$ to ensure that particles and antiparticles decay both at positive infinite times.

For a massive vector meson with a gauge fixing term in the action [see (5.545)], the matrix (5.582) becomes

$$L_{\mu\nu}(k) = (k^2 - M^2)P_{T\,\mu\nu}(k) + \left(\frac{k^2}{\alpha} - M^2\right)P_{L\,\mu\nu}(k), \tag{5.585}$$

and the inverse (5.583):

$$\begin{aligned} L^{-1\,\mu\nu}(k) &= \frac{1}{k^2-M^2}P_T^{\mu\nu}(k) + \frac{\alpha}{k^2-\alpha M^2}P_L^{\mu\nu}(k) \\ &= \frac{1}{k^2-M^2}\left[g^{\mu\nu} - (1-\alpha)\frac{k^\mu k^\nu}{k^2-\alpha M^2}\right], \end{aligned} \tag{5.586}$$

Due to the Schwinger term, the propagator is different from the Green function associated with the field equation (5.542). In Chapters 7, 8, and 10 we shall see that when interactions are present, there are two ways of evaluating the physical consequences. One of them is based on the interaction picture of quantum mechanics and leads to a Schwinger-Dyson perturbation expansion for scattering amplitudes, the other makes use of functional integrals and leads to a similar expansion. The first is based on a Hamiltonian approach in which the propagator plays a central role and interactions are described by an interaction Hamiltonian, in the second the action is relevant and covariant Green functions replace the propagators. The results are of course the same in both cases, as we shall see. The cancelation of all effects of the Schwinger term is caused by the last term in the interaction Hamiltonian density derived in Eq. (5.568).

The commutator of two vector fields is

$$[V^{\mu\dagger}(x), V^{\nu}(x')] \;=\; C^{\mu\nu}(x-x'), \tag{5.587}$$

with

$$\begin{aligned} C^{\mu\nu}(x-x') &= \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-x')}\, 2\pi\epsilon(k^0)\delta(k^2-M^2)\left(-g^{\mu\nu}+\frac{k^\mu k^\nu}{M^2}\right) \\ &= \left(-g^{\mu\nu}-\frac{\partial^\mu\partial^\nu}{M^2}\right) C(x-x').. \end{aligned} \tag{5.588}$$

At equal times, we rewrite in the integrand

$$\delta(k^2-M^2) = \frac{1}{2\omega_{\mathbf{k}}}[\delta(k^0-\omega_{\mathbf{k}})+\delta(k^0+\omega_{\mathbf{k}})],$$

with $\omega_{\mathbf{k}} \equiv \sqrt{\mathbf{k}^2+M^2}$ and see that because of the oddness of $\epsilon(k^0)$, the commutator vanishes, except for $(\mu,\nu)=(0,i)$, where $k^0\epsilon(k^0)=\omega_{\mathbf{k}}$. produces an even integrand leading to the initial canonical commutation relation (5.551).

Let us end this section by justifying the earlier-used $i\eta$-prescription in the propagator (5.524) of the photon field. For this we add a mass term to the electromagnetic Lagrangian (5.361) with the gauge-fixing Lagrangian, which leads to a massive vector photon Lagrangian

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}M^2 A_\mu A^\mu - D(x)\partial^\mu A_\mu(x) + \frac{\alpha}{2}D^2(x), \qquad \alpha \geq 0. \tag{5.589}$$

The Euler-Lagrange equations are now [compare (5.366)]

$$\left[(-\partial^2-M^2)g_{\mu\nu} + \left(1-\frac{1}{\alpha}\right)\partial_\mu\partial_\nu\right] A^\nu(x) = 0, \tag{5.590}$$

so that the propagator in momentum space obeys the equation

$$\left[(k^2-M^2)g_{\mu\nu} - \left(1-\frac{1}{\alpha}\right)k_\mu k_\nu\right] G^{\nu\kappa}(k) = -i\delta^\mu{}_\kappa. \tag{5.591}$$

The matrix on the left-hand side is decomposed into transverse and longitudinal parts as

$$L_{\mu\nu}(k) = (k^2-M^2)P_{T\,\mu\nu}(k) + \frac{1}{\alpha}\left(k^2-\alpha M^2\right)P_{L\,\mu\nu}(k), \tag{5.592}$$

from which we obtain the inverse

$$\begin{aligned} L^{-1\,\mu\nu}(k) &= \frac{1}{k^2-M^2}P_T^{\mu\nu}(k) + \frac{\alpha}{k^2-\alpha M^2}P_L^{\mu\nu}(k), \\ &= \frac{1}{k^2-M^2}\left(g^{\mu\nu}-\frac{k^\mu k^\nu}{k^2}\right) + \frac{\alpha}{k^2-\alpha M^2}\frac{k^\mu k^\nu}{k^2}, \end{aligned} \tag{5.593}$$

which can be rearranged to

$$L^{-1\,\mu\nu}(k) \;=\; \frac{g^{\mu\nu}}{k^2-M^2}+(\alpha-1)\frac{k^\mu k^\nu}{(k^2-\alpha M^2)(k^2-M^2)}, \tag{5.594}$$

so that (5.532) is solved by the matrix

$$G^{\mu\nu}(k)=-iL^{-1\,\mu\nu}(k). \tag{5.595}$$

The condition $\alpha > 0$ in the Lagrangian (5.589) ensures that both poles in the second denominator lie at a physical mass square.

Adding to the mass an infinitesimal imaginary parts $-i\eta$ with $\alpha > 0$, and letting $M \to 0$ we obtain precisely the $i\eta$-prescription of Eq. (5.524).

5.5.4 Behavior under Discrete Symmetry Transformations

Under the discrete transformations P, T, and C, a massive vector field transforms in the same way as the vector potential of electromagnetism in Eqs. (5.533)–(5.537), except for different possible phases η_P, η_T, η_C.

In the second-quantized Hilbert space, these amount to the following transformation laws for the creation and annihilation operators of particles of helicity λ. Under parity:

$$\mathcal{P}a^\dagger_{\mathbf{k},\lambda}\mathcal{P}^{-1} \;\equiv\; a'^\dagger_{\mathbf{k},\lambda}=\eta_P a^\dagger_{-\mathbf{k},-\lambda}, \tag{5.596}$$

with $\eta_P = \pm 1$. Under time reversal:

$$\mathcal{T}a^\dagger_{\mathbf{k},\lambda}\mathcal{T}^{-1} \;\equiv\; a'^\dagger_{\mathbf{k},\lambda}=\eta_T a^\dagger_{-\mathbf{k},\lambda}, \tag{5.597}$$

with an arbitrary phase factor η_T, and under charge conjugation

$$\mathcal{C}a^\dagger_{\mathbf{k},\lambda}\mathcal{C}^{-1} \;\equiv\; a'^\dagger_{\mathbf{k},\lambda}=\eta_C a^\dagger_{\mathbf{k},\lambda}, \tag{5.598}$$

with $\eta_C = \pm 1$.

Vector mesons such as the ρ-meson of mass $m_\rho \approx 759$ MeV and the ω-meson of mass $m_\omega \approx 782$ MeV transform with the three phase factors η_P, η_T, η_C being equal to those of a photon. This is a prerequisite for the theory of *vector meson dominance* of electromagnetic interactions which approximate all electromagnetic interactions of strongly interacting particles by assuming the photon to become a mixture of a neutral ρ- and an ω-meson, which then undergo strong interactions.

We omit the calculation of the Hamilton operator since the result is an obvious generalization of the previous expression (5.571) for neutral vector bosons:

$$H=\sum_{\mathbf{p}}p^0\sum_{\lambda=\pm1,0}\left(a^\dagger_{\mathbf{p},\lambda}a_{\mathbf{p},\lambda}-b_{\mathbf{p},\lambda}b^\dagger_{\mathbf{p},\lambda}\right)=\sum_{\mathbf{p}}p^0\sum_{s_3=\pm1,0}\left(a^\dagger_{\mathbf{p},s_3}a_{\mathbf{p},s_3}-b_{\mathbf{p},s_3}b^\dagger_{\mathbf{p},s_3}\right). \tag{5.599}$$

5.6 SPIN-3/2 FIELDS

The Rarita-Schwinger field of massive spin-3/2 particles is expanded just like (5.211) as follows:

$$\psi_\mu(x) = \sum_{\mathbf{p},S_3} \frac{1}{\sqrt{Vp^0/M}} \left[e^{-ipx} u_\mu(\mathbf{p}, S_3) a_{\mathbf{p},S_3} + e^{ipx} v_\mu(\mathbf{p}, S_3) b^\dagger(\mathbf{p}, S_3) \right]. \tag{5.600}$$

where the spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(\mathbf{p}, S_3)$ are solutions of equations analogous to (3.602):

$$L^{\mu\nu}(p) u_\nu(\mathbf{p}, S_3) = 0, \tag{5.601}$$

$$L^{\mu\nu}(-p) v_\nu(\mathbf{p}, S_3) = 0, \tag{5.602}$$

where $L^{\mu\nu}(p)$ is the Fourier-transformed differential operator (3.890) with positive mass shell energy $p^0 = \sqrt{\mathbf{p}^2 + M^2}$. The Rarita-Schwinger spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(\mathbf{p}, S_3)$ can be constructed explicitly from those of spin 1/2 and the polarization vectors (3.342) of spin 1 with the help of the Clebsch-Gordan coefficients on Table 3.2:

$$u_\mu(\mathbf{p}, S_3) = \sum_{s_3,s_3'} \langle \tfrac{3}{2}, S_3 | 1, s_3; \tfrac{1}{2}, s_3' \rangle \epsilon_\mu(\mathbf{p}, s_3) u(\mathbf{p}, s_3'), \tag{5.603}$$

$$v_\mu(\mathbf{p}, S_3) = \sum_{s_3,s_3'} \langle \tfrac{3}{2}, S_3 | 1, s_3; \tfrac{1}{2}, s_3' \rangle \epsilon_\mu(\mathbf{p}, s_3) v(\mathbf{p}, s_3'). \tag{5.604}$$

The calculation of the propagator

$$S_{\mu\nu}(x, x') = \langle 0 | T \psi_\mu(x) \bar{\psi}_\nu(x') | 0 \rangle \tag{5.605}$$

is now somewhat involved. As in the case of spin-zero, spin-1/2, and massive spin-1 fields, the result can be derived most directly by inverting the matrix $L_{\mu\nu}(p)$. For this we make use of the fact that for reasons of covariance, ${L^{-1}}_{\mu\nu}$ may be expanded into the tensors $g_{\mu\nu}, \gamma_\mu\gamma_\nu, \gamma_\mu p_\nu, \gamma_\nu p_\mu, p_\mu p_\nu$ with coefficients of the form $A + B\not{p}$. By multiplying this expansion with $L^{\nu\lambda}(p)$ and requiring the result to be equal to ${\delta_\mu}^\lambda$, we find ${L^{-1}}_{\mu\nu}$ is equal to the 4×4 spinor matrix

$$\begin{aligned} {L^{-1}}_{\mu\nu} = \Bigg\{ & \frac{\not{p} + M}{p^2 - M^2} \left[-g_{\mu\nu} + \frac{1}{3}\gamma_\mu\gamma_\nu + \frac{1}{3M}(\gamma_\mu p_\nu - \gamma_\nu p_\mu) + \frac{2}{3}\frac{p_\mu p_\nu}{M} \right] \\ & - \frac{1}{6M^2} \frac{w+1}{(2w+1)^2} \left[(4w+2)\gamma_\mu p_\nu + (w+1)\not{p}\gamma_\mu\gamma_\nu + 2w p_\mu \gamma_\nu - 2wM\gamma_\mu\gamma_\nu \right] \Bigg\}. \end{aligned} \tag{5.606}$$

For simplicity, we have given this matrix only for the case $w =$ real. In analogy with (5.276), the propagator is equal to the Fourier transform of ${L^{-1}}_{\mu\nu}(p)$:

$$S_{\mu\nu}(x, x') = \int \frac{d^4p}{(2\pi)^4} {L^{-1}}_{\mu\nu}(p) e^{-ip(x-x')}. \tag{5.607}$$

The wave equation has a nontrivial solution where $L^{-1}(p)$ has a singularity. From (5.606) we see that this happens only on the positive- and negative-energy mass shells at

$$p^0 = \pm\sqrt{\mathbf{p}^2 + M^2}. \tag{5.608}$$

By writing the prefactor in (5.606) as

$$\frac{\not p + M}{p^2 - M^2} = \frac{1}{\not p - M}, \tag{5.609}$$

we see that only solutions of

$$(\not p - M)_\alpha{}^{\alpha'}\psi_{\mu\alpha'}(p) = 0, \quad p^0 = \pm\sqrt{\mathbf{p}^2 + M^2} \tag{5.610}$$

can cause this singularity. These are the spinors $u_\mu(\mathbf{p}, S_3)$ and $v_\mu(-\mathbf{p}, S_3)$, respectively. The residue matrix accompanying the singularity is independent of the parameter c. It must have the property of projecting precisely into the subspace of $\psi_{\mu\alpha}(p)$ in which the wave equation $L^{\mu\nu}(p)\psi_\nu(p) = 0$ is satisfied. Let

$$L^{-1\,\mu\nu}(p) = \frac{2M}{p^2 - M^2}P^{\mu\nu}(p) + \text{regular piece}. \tag{5.611}$$

After a little algebra we find

$$P^{\mu\nu}(p) = \frac{\not p + M}{2M}\left[-g_{\mu\nu} + \frac{1}{3}\gamma_\mu\gamma_\nu + \frac{1}{3M}(p_\mu\gamma_\nu - p_\nu\gamma_\mu) + \frac{2}{3}\frac{p_\mu p_\nu}{M^2}\right]. \tag{5.612}$$

The residue matrix $P^{\mu\nu}(p)$ is uniquely fixed only on for p_0 on the upper and lower mass shells $p_0 = \pm\sqrt{\mathbf{p}^2 + M^2}$. There it has the form $P_\pm^{\mu\nu}(\mathbf{p})$, respectively. The expression (5.612) is a common covariant off-shell extension of these two matrices.

These matrices and their extension $P^{\mu\nu}(p)$ are independent of the parameter c. They are projection matrices, satisfying

$$P^{\mu\nu}g_{\nu\kappa}P^{\kappa\lambda} = P^{\mu\lambda}. \tag{5.613}$$

It is easy to verify that for $p^2 = M^2$, the matrix $P_{\mu\nu}(\mathbf{p})$ satisfies the same equations as the Rarita-Schwinger spinors $u_\mu(\mathbf{p}, S_3)$

$$(\not p - M)P_{\mu\nu}(p) = 0, \tag{5.614}$$
$$P_{\mu\nu}(p)p^\nu = 0, \tag{5.615}$$
$$P_{\mu\nu}(p)\gamma^\nu = 0. \tag{5.616}$$

For this reason, $P_{\mu\nu}(\pm p)$ with $p^0 = \omega_\mathbf{p}$ can be expanded as

$$P_{\mu\nu}(p) = \sum_{s_3} u_\mu(\mathbf{p}, S_3)\bar u_\nu(\mathbf{p}, S_3), \tag{5.617}$$
$$P_{\mu\nu}(-p) = -\sum_{s_3} v_\mu(\mathbf{p}, S_3)\bar v_\nu(\mathbf{p}, S_3). \tag{5.618}$$

The projection matrix is equal to the polarization sums of the spinors $u_\mu(\mathbf{p},S_3)$ and $v_\mu(\mathbf{p},S_3)$, except for a minus sign accounting for the fact that $\bar{v}(\mathbf{p},S_3)v(\mathbf{p},S_3) = -\bar{u}(\mathbf{p},S_3)u(\mathbf{p},S_3)$, just as in the Dirac case [recall the discussion after Eq. (3.644)].

The behavior under discrete symmetry transformations of the creation and annihilation operators of a Rarita-Schwinger field is the same as that of a product of a Dirac operator and a massive vector meson operator, i.e., it is given by a combination of the transformation laws (5.288), (5.310), (5.293) and (5.596), (5.597), and (5.598).

5.7 GRAVITONS

In order to quantize the gravitational field we first have to rewrite the action in terms of squares of first derivative terms. After a partial integration, it reads

$$\mathcal{A} = \frac{1}{8\kappa}\int d^4x \left[\partial_\lambda h^{\mu\nu}\partial^\lambda h_{\mu\nu} - 2\partial^\nu h^{\mu\lambda}\partial_\lambda h_{\mu\nu} + 2\partial_\mu h\partial_\nu h^{\mu\nu} - \partial_\mu h\partial_\nu h\right], \tag{5.619}$$

where $h \equiv h^\mu{}_\mu$. A few further partial integrations brings this to the alternative form

$$\mathcal{A} = \int d^4x\, \mathcal{L}(x) = \frac{1}{2}\int d^4x\, \pi_{\lambda\mu\nu}\partial_\lambda h_{\mu\nu}, \tag{5.620}$$

where

$$\pi_{\lambda\mu\nu} \equiv \frac{1}{8\kappa}\left[\partial_\lambda h_{\mu\nu} - \partial_\mu h_{\lambda\mu} + g_{\lambda\nu}\partial_\mu h - g_{\mu\nu}\partial_\lambda h + g_{\mu\nu}\partial^\kappa h_{\kappa\lambda} - g_{\lambda\nu}\partial^\kappa h_{\kappa\mu}\right] + (\mu \leftrightarrow \nu) \tag{5.621}$$

is defined by

$$\pi_{\lambda\mu\nu}(x) \equiv \frac{\partial\mathcal{L}(x)}{\partial[\partial_\lambda h_{\mu\nu}(x)]}. \tag{5.622}$$

It is antisymmetric in $\lambda\mu$ and symmetric in $\mu\nu$. The components $\pi_{0\mu\nu}$ play the role of the canonical field momenta. Similar to the electromagnetic case, four of the six independent components π_{0ij} vanish, as a consequence of the invariance of the action under gauge transformations (3.357):

$$h_{\mu\nu}(x) \to h_{\mu\nu}(x) + \partial_\mu\Lambda_\nu(x) + \partial_\nu\Lambda_\mu(x). \tag{5.623}$$

Going over to the field $\phi_{\mu\nu}(x)$ of Eq. (3.362) and the Hilbert gauge (3.362), we expand the field into plane waves e^{-ikx} with $k^0 = |\mathbf{k}|$ and two transverse polarization tensors (3.362):

$$\phi^{\mu\nu}(x) = \frac{1}{\sqrt{2Vp^0}}\sum_{\mathbf{k}}\sum_{\lambda=\pm 2}\left[a_{\mathbf{k},\lambda}\epsilon^{\mu\nu}(\mathbf{k},\lambda)e^{-ikx} + a^\dagger_{\mathbf{k},\lambda}\epsilon^{\mu\nu *}(\mathbf{k},\lambda)e^{ikx}\right], \tag{5.624}$$

The behavior under discrete symmetry transformations of the creation and annihilation operators of a free graviton field is the same as that of a product of two photon operators in Eqs. (5.533)–(5.535).

5.8 SPIN-STATISTICS THEOREM

When quantizing Klein-Gordon and Dirac fields we directly used commutation rules for spin 0 and anticommutation rules for spin 1/2. In nonrelativistic quantum field theory this procedure was dictated by experimental facts. It is one of the important successes of relativistic quantum field theory that this connection between spin and statistics is a necessity if one wants to quantize free fields canonically. Let us first look at the real scalar field theory, and consider the field commutator expanded as in (5.11):

$$\begin{aligned} &i[\partial^0\phi(\mathbf{x},t),\phi(\mathbf{x}',t)] \\ &\quad=\sum_{\mathbf{p},\mathbf{p}'}\frac{1}{\sqrt{2Vp^0 2Vp^{0'}}}\left(e^{i(\mathbf{px}-\mathbf{p}'\mathbf{x}'))}p^0[a_{\mathbf{p}},a^\dagger_{\mathbf{p}'}]+e^{-i(\mathbf{px}-\mathbf{p}'\mathbf{x}'))}(-p^0)[a^\dagger_{\mathbf{p}},a_{\mathbf{p}'}]\right), \end{aligned} \tag{5.625}$$

where we have left out terms with vanishing commutators $[a_{\mathbf{p}},a_{\mathbf{p}'}]$ and $[a^\dagger_{\mathbf{p}},a^\dagger_{\mathbf{p}'}]$. Inserting the commutators (5.15), we see that both contributions just add up correctly to give a δ-function, as they should to fulfill the canonical field commutation rules (5.2)–(5.4). Suppose now for a moment that the particles were to obey Fermi statistics. Then the symbols [,] would stand for anticommutators, and the two contributions would have to be subtracted from each other and give zero. Thus a real relativistic scalar field cannot be quantized according to the wrong Fermi statistics. The situation is similar for a complex scalar field, where we obtain

$$\begin{aligned} &i[\partial^0\phi(\mathbf{x},t),\phi^\dagger(\mathbf{x}',t)] \\ &\quad=\sum_{\mathbf{p},\mathbf{p}'}\frac{1}{\sqrt{2Vp^0 2Vp^{0'}}}\left(e^{i(\mathbf{px}-\mathbf{p}'\mathbf{x}')}p^0[a_{\mathbf{p}},a^\dagger_{\mathbf{p}'}]+e^{-i(\mathbf{px}-\mathbf{p}'\mathbf{x}')}(-p^0)[b^\dagger_{\mathbf{p}},b_{\mathbf{p}'}]\right), \end{aligned} \tag{5.626}$$

where all those commutators have been omitted which vanish. Again, the two terms add up correctly to give a δ-function while the use of anticommutators would lead to a vanishing of the right-hand side.

These observations are related to another remark made earlier when we expanded the free complex field into the solutions of the wave equation and wrote down immediately creation operators $b^\dagger_{\mathbf{p}}$ for the negative energy solutions e^{ipx} as a generalization of $a^\dagger_{\mathbf{p}}$ for the real field. At that place we could, in principle, have had the option of using $b_{\mathbf{p}}$. But looking at (5.626) we realize that this would not have led to canonical commutation rules in either statistics.

Consider now the case of spin-1/2 fields. Here we calculate the anticommutator expanded via (5.210):

$$\begin{aligned} \left\{\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t)\right\}&=\sum_{\mathbf{p},\mathbf{p}'}\frac{1}{\sqrt{Vp^0/M}\sqrt{Vp^{0'}/M}}\sum_{s_3,s_3'=\pm1/2} \\ &\times\left[e^{i(\mathbf{px}-\mathbf{p}'\mathbf{x}')}\left\{a_{\mathbf{p},s_3},a^\dagger_{\mathbf{p}',s_3'}\right\}u(\mathbf{p},s_3)u^\dagger(\mathbf{p}'s_3')\right. \\ &\left.+\,e^{-i(\mathbf{px}-\mathbf{p}'\mathbf{x}')}\left\{b^\dagger_{\mathbf{p},s_3},b_{\mathbf{p},s_3'}\right\}v(\mathbf{p},s_3)v^\dagger(\mathbf{p}',s_3')\right]. \end{aligned} \tag{5.627}$$

We now use the anticommutation rules (5.215) and (5.216)

$$\begin{aligned}\left\{a_{\mathbf{p},s_3}, a^\dagger_{\mathbf{p}',s_3'}\right\} &= \delta_{\mathbf{p},\mathbf{p}'}\delta_{s_3,s_3'}, \\ \left\{b^\dagger_{\mathbf{p},s_3}, b_{\mathbf{p}',s_3'}\right\} &= \delta_{\mathbf{p},\mathbf{p}'}\delta_{s_3,s_3'},\end{aligned} \tag{5.628}$$

and the polarization sums (3.641) (3.642),

$$\begin{aligned}\sum_{s_3} u(\mathbf{p},s_3)u^\dagger(\mathbf{p},s_3) &= \frac{\not p + M}{2M}\gamma_0, \\ \sum_{s_3} v(\mathbf{p},s_3)v^\dagger(\mathbf{p},s_3) &= \frac{\not p - M}{2M}\gamma_0,\end{aligned} \tag{5.629}$$

to find

$$\left\{\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t)\right\} = \sum_{\mathbf{p}} \frac{1}{Vp^0/M}\left(e^{-ip(x-x')}\frac{\not p + M}{2M}\gamma_0 + e^{ip(x-x')}\frac{\not p - M}{2M}\gamma_0\right). \tag{5.630}$$

The δ-function arises after a cancellation of the terms M and $\mathbf{p}\boldsymbol{\gamma}$ in the numerator from the sum of the $p^0\gamma^0$ -terms.

Let us see what would happen if we use commutators for quantization and thus the wrong particle statistics. Then the $[b^\dagger_{\mathbf{p},s_3}, b_{\mathbf{p},s_3}]$ -term would change its sign and fail to produce the desired δ-function. At first sight, one might want to correct this by using in the expansion of $\psi(\mathbf{x},t)$ annihilation operators $d_{\mathbf{p},s_3}$ rather than a creators $b^\dagger_{\mathbf{p},s_3}$. Then the commutator $[b^\dagger_{\mathbf{p},s_3}, b_{\mathbf{p},s_3}]$ would be replaced by $[d_{\mathbf{p},s_3}, d^\dagger_{\mathbf{p},s_3}]$, and give indeed a correct sign after all!

However, the problem would then appear at a different place. When calculating the energy, we found in (5.599)

$$H = \sum_{\mathbf{p},s_3} p^0\left(a^\dagger_{\mathbf{p},s_3}a_{\mathbf{p},s_3} - b_{\mathbf{p},s_3}b^\dagger_{\mathbf{p},s_3}\right), \tag{5.631}$$

independent of statistics. Changing $b_{\mathbf{p},s_3}$ to $d^\dagger_{\mathbf{p},s_3}$ in the field expansion would give, instead,

$$H = \sum_{\mathbf{p},s_3} p^0\left(a^\dagger_{\mathbf{p},s_3}a_{\mathbf{p},s_3} - d^\dagger_{\mathbf{p},s_3}d_{\mathbf{p},s_3}\right). \tag{5.632}$$

But this is an operator whose eigenvalues can take arbitrarily large negative values on states containing a large number of creation operators $d^\dagger_{\mathbf{p},s_3}$ in front of the vacuum state $|0\rangle$. Such an energy is unphyical since it would imply the existence of a perpetuum mobile.

The spin-statistics relation can be extended in a straightforward way to vector and tensor fields, and further to fields of any spin s, For each of these fields, quantization with the wrong statistics would imply either a failure of locality or of the positivity of the energy.

We shall sketch the general proof only for the spinor field $\xi(x)$ introduced in Section 3.19. This is expanded into plane waves (3.19) as before, assigning creation operators of antiparticles to the Fourier components of the negative-energy solutions:

$$\xi(x) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2Vp^0}} \left[e^{-ipx} w(\mathbf{p}, s_3) a_{\mathbf{p},s_3} + e^{ipx} w^c(\mathbf{p}, s_3)\, b^\dagger_{\mathbf{p},s_3} \right]. \tag{5.633}$$

Here

$$w^c(\mathbf{p}, s_3) = c^{\{2s\}} w^*(\mathbf{p}, s_3) = w(\mathbf{p}, s_3') c^{(s)}_{s_3',s_3} = w(\mathbf{p}, -s_3)(-1)^{s-s_3} \tag{5.634}$$

are the charge-conjugate spinors. The matrices $c^{\{2s\}}$ have the labels $c^{\{2s\}}_{n_1,n_2;n_1',n_2'}$, and are equivalent to the matrices $c^{(s)}_{s_3,s_3'}$ reversing the spin direction by a rotation around the y-axis by an angle π [recall the defining equation (3.835)]. The relation between their indices n_1, n_2 and s_3 is the same as in the rest spinors (3.873). These matrices have the property

$$c^{\{2s\}} c^{\{2s\}\dagger} = 1, \qquad \left(c^{\{2s\}} \right)^2 = (-1)^{2s}. \tag{5.635}$$

The commutation or anticommutation relation between two such spinor fields has the form

$$\begin{aligned} i[\phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t')]_\mp &= \sum_{\mathbf{p}} \frac{1}{2Vp^0} \left[e^{-ip(x-x')} \sum_{s_3} w(\mathbf{p}, s_3) w^*(\mathbf{p}, s_3) \right. \\ &\qquad \left. \pm e^{ip(x-x')} \sum_{s_3} w^c(\mathbf{p}, s_3) w^{c*}(\mathbf{p}, s_3) \right], \end{aligned} \tag{5.636}$$

Recalling the polarization sum (3.875),

$$P(p) \equiv \sum_{s_3} w^{\{2s\}}(\mathbf{p}, s_3) w^{\{2s\}*}(\mathbf{p}, s_3) = \left(\frac{p\sigma}{M} \right)^{\{2s\}}, \tag{5.637}$$

and noting that the charge-conjugate spinors have the same sum, this becomes

$$i[\phi(\mathbf{x}, t), \phi^\dagger(\mathbf{x}', t')]_\mp = \sum_{\mathbf{p}} \frac{1}{2Vp^0} P(p) \left[e^{-ip(x-x')} \mp e^{ip(x-x')} \right]. \tag{5.638}$$

The polarization sum $P(p)$ is a homogenous polynomial in p^0 and $\mathbf{p}$ of degree $2s$. It has therefore the symmetry property $P(-p) = (-1)^{2s} P(p)$. The energy p^0 lies on the mass shell $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2}$. Replacing all even powers $\omega_{\mathbf{p}}^{2n}$ by $(\mathbf{p}^2 + M^2)^n$, and all odd powers $\omega_{\mathbf{p}}^{2n+1}$ by $\omega_{\mathbf{p}}(\mathbf{p}^2 + M^2)^n$, we obtain for $P(p)$ the following generic dependence on the spatial momenta

$$P(p) = P_0(\mathbf{p}) + \omega_{\mathbf{p}} P_1(\mathbf{p}), \tag{5.639}$$

where $P_0(\mathbf{p})$ and $P_1(\mathbf{p})$ are polynomials of $\mathbf{p}$ with the reflection properties

$$P_0(-\mathbf{p}) = (-1)^{2s} P_0(\mathbf{p}), \qquad P_1(-\mathbf{p}) = -(-1)^{2s} P_1(\mathbf{p}). \tag{5.640}$$

Thus we can write

$$i[\phi(\mathbf{x},t),\phi^\dagger(\mathbf{x}',t')]_\mp \tag{5.641}$$
$$=\sum_{\mathbf{p}}\frac{1}{2Vp^0}\left\{\left[P_0(\mathbf{p})+p^0P_1(\mathbf{p})\right]e^{-ip(x-x')}\mp(-1)^{2s}\left[P_0(-\mathbf{p})-p^0P_1(-\mathbf{p})\right]e^{ip(x-x')}\right\}.$$

After replacing $\pm\mathbf{p}$ by spatial derivatives $-i\boldsymbol{\nabla}$, the momentum-dependent factors can be taken outside the momentum sums, and we obtain

$$\begin{aligned} i[\phi(\mathbf{x},t),\phi^\dagger(\mathbf{x}',t')]_\mp &= P_0(-i\boldsymbol{\nabla})\sum_{\mathbf{p}}\frac{1}{2Vp^0}\left[e^{-ip(x-x')}\mp(-1)^{2s}e^{ip(x-x')}\right] \\ &+ P_1(-i\boldsymbol{\nabla})\sum_{\mathbf{p}}\frac{1}{2V}\left[e^{-ip(x-x')}\pm(-1)^{2s}e^{ip(x-x')}\right]. \end{aligned} \tag{5.642}$$

In the limit of infinite volume, the right-hand side becomes [recall (5.44)]

$$\begin{aligned} &P_0(-i\boldsymbol{\nabla})\left[G^{(+)}(x-x')\mp(-1)^{2s}G^{(+)}(x-x')\right] \\ +\;&P_1(-i\boldsymbol{\nabla})\left[G^{(+)}(x-x')\pm(-1)^{2s}G^{(+)}(x-x')\right]. \end{aligned} \tag{5.643}$$

At equal times, this reduces to

$$\begin{aligned} &P_0(-i\boldsymbol{\nabla})[1\mp(-1)^{2s}]\,G^{(+)}(\mathbf{x}-\mathbf{x}',0) \\ &+P_1(-i\boldsymbol{\nabla})[1\pm(-1)^{2s}]\,\delta^{(3)}(\mathbf{x}-\mathbf{x}'). \end{aligned} \tag{5.644}$$

Locality requires that the commutator at spacelike distances vanishes. Since $G^{(+)}(\mathbf{x}-\mathbf{x}',0)\neq 0$, the prefactor of the first term must be zero, and hence

$$(-1)^{2s}=\left\{\begin{array}{rl} 1 & \text{for bosonic commutators,} \\ -1 & \text{for fermionic anticommutators.}\end{array}\right. . \tag{5.645}$$

This proves the spin-statistics relation for spin-s spinor fields $\xi(x)$.

Note that the locality of the free fields always forces particles and antiparticles to have the same mass and spin.

5.9 CPT THEOREM

All of the above local free-field theories have a universal property under the discrete symmetry operations C, P, and T. When being subjected to a product CPT of the three operations, the Lagrangian is invariant. We shall see later in Chapter 24, that this remains true also in the presence of interactions, as long as these are local and Lorentz-invariant.

When introducing local interactions between local fields they will always have the property of being invariant under the operation CPT. This is the content of the so-called CPT-theorem.[29] This property guarantees that the equality of masses and spins of particles and antiparticles remains true also in the presence of interactions. If there is a mass difference in nature, it must be extremely small. Direct measurements of masses of electrons and protons and their antiparticles are too insensitive to detect a difference with present experiments.

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[29] W. Pauli, *Niels Bohr and the Development of Physics*, McGraw-Hill, N.Y., 1955; G. Lüders, Ann. Phys. N.Y. **2**, 1 (1957); as well as the predecessors J. Schwinger, Phys. Rev. **82**, 664 (1951); **82**, 914 (1951); Proc. Nat. Acad. Sciences (USA), **37**, 452 (1951).

5.10 PHYSICAL CONSEQUENCES OF VACUUM FLUCTUATIONS — CASIMIR EFFECT

For each of the above relativistic quantum fields we have found an infinite vacuum energy due to the *vacuum fluctuations* of the field. For a real scalar field, this energy is [see (5.31)]

$$E_0 = \frac{1}{2}\sum_{\mathbf{k}} k^0 = \frac{1}{2}\sum_{\mathbf{k}} \omega_{\mathbf{k}} = \frac{\hbar c}{2}\sum_{\mathbf{k}} \sqrt{\mathbf{k}^2 + c^2M^2/\hbar^2}, \tag{5.646}$$

where $\mathbf{k} = \mathbf{p}/\hbar$ are the wave vectors. In many calculations, this energy is irrelevant and discarded. There are, however, important physical phenomena where this is impossible, since their origin lies in the vacuum energy (5.646). One of them is the cosmological constant as discussed on p. 278. The other appears in electromagnetism and is observabel in the form of *Van der Waals forces*) between different dielectric media,

In the present context of free fields in a vacuum, the most interesting phenomenon is the *Casimir effect*. Vacuum fluctuations of electromagnetic fields cause an attraction between two parallel closely spaced silver plates in an otherwise empty space. The basic electromagnetic property of a silver plate is to enforce the vanishing of the parallel electric field at its surface, due to the high conductivity. Let us study a specific situation and suppose the silver plates to be parallel to the xy-plane one at $z = 0$ and the other at $z = d$. To have discrete momenta the whole system is imagined to be enclosed in a very large conducting box

$$x \in (-L_x/2, L_x/2), \qquad y \in (-L_y/2, L_y/2), \qquad , z \in (-L_z/2, L_z/2). \tag{5.647}$$

The plates divide the box into a thin slice of volume $L_x\ L_y\ d$ and two large pieces of volumes $L_y\ L_yL_z/2$ below and $L_xL_y(L_z/2 - d)$ above the slice (see Fig. 5.5). These are three typical resonant cavities of classical electrodynamics. For waves of frequency ω, the Maxwell equations $\partial_\mu F^{\mu\nu} = 0$ read, in natural units with $c = 1$ [recall (3.238)],

$$\boldsymbol{\nabla} \times \mathbf{B} = \dot{\mathbf{E}} = -i\omega\mathbf{E}, \qquad \boldsymbol{\nabla} \cdot \mathbf{E} = 0. \tag{5.648}$$

Since the field components parallel to the conducting surface vanish, the first equation implies that the same is true for the magnetic field components normal to the surface. Inserting the equations into each other, and using the other two Maxwell

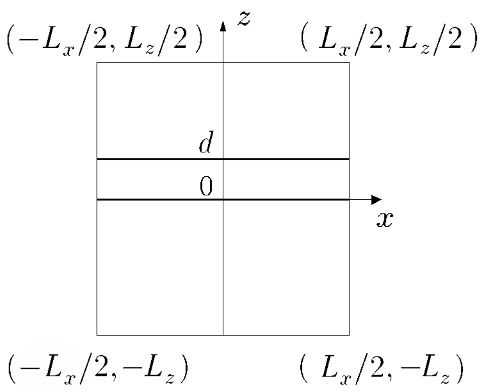

FIGURE 5.5 Geometry of the plates for the calculation of the Casimir effect.

equations [recall (3.238)] following from the Bianchi identity $\partial_\mu \tilde{F}^{\mu\nu} = 0$ [recall (3.237)]:

$$\boldsymbol{\nabla} \times \mathbf{E} = i\omega \mathbf{B}, \qquad \boldsymbol{\nabla} \cdot \mathbf{B} = 0. \tag{5.649}$$

the fields $\mathbf{E}$ and $\mathbf{B}$ are both seen to satisfy the *Helmholtz equations*

$$\left(\boldsymbol{\nabla}^2 + \omega^2\right) \left\{ \begin{array}{c} \mathbf{E}(\mathbf{x}) \\ \mathbf{B}(\mathbf{x}) \end{array} \right\} = 0. \tag{5.650}$$

They are solved by the ansatz

$$\left\{ \begin{array}{c} \mathbf{E}(\mathbf{x}) \\ \mathbf{B}(\mathbf{x}) \end{array} \right\} = \left\{ \begin{array}{c} \mathbf{E}_0(\mathbf{x}_\perp) \\ \mathbf{B}_0(\mathbf{x}_\perp) \end{array} \right\} e^{ik_z z}, \tag{5.651}$$

where $\mathbf{x}_\perp \equiv (x, y)$ are the components of $\mathbf{x}$ parallel to the plates. The fields $\mathbf{E}_0(\mathbf{x}_\perp)$, $\mathbf{B}_0(\mathbf{x}_\perp)$ satisfy the differential equation

$$\left(\boldsymbol{\nabla}_\perp{}^2 + \omega^2 - k_z{}^2\right) \left\{ \begin{array}{c} \mathbf{E}_0(\mathbf{x}_\perp) \\ \mathbf{B}_0(\mathbf{x}_\perp) \end{array} \right\} = 0, \tag{5.652}$$

where $\boldsymbol{\nabla}_\perp$ is the transverse derivative

$$\boldsymbol{\nabla}_\perp \equiv (\nabla_x, \nabla_y, 0). \tag{5.653}$$

We now split the original fields $\mathbf{E}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x})$ into a component parallel and orthogonal to the unit vector $\hat{z}$ along the z-axis:

$$\begin{aligned} \mathbf{E} &= E_z \hat{\mathbf{z}} + \mathbf{E}_\perp \\ \mathbf{B} &= B_z \hat{\mathbf{z}} + \mathbf{B}_\perp, \end{aligned} \tag{5.654}$$

and see that the Maxwell equations (5.648) can be solved for $\mathbf{E}_\perp, \mathbf{B}_\perp$ in terms of E_z, B_z:

$$\begin{aligned} \mathbf{B}_\perp &= \frac{1}{\omega^2 + \boldsymbol{\nabla}^2} \left[\boldsymbol{\nabla}_\perp \partial_z B_z + i\omega \hat{\mathbf{z}} \times \boldsymbol{\nabla}_\perp E_z\right], \\ \mathbf{E}_\perp &= \frac{1}{\omega^2 + \boldsymbol{\nabla}^2} \left[\boldsymbol{\nabla}_\perp \partial_z E_z - i\omega \hat{\mathbf{z}} \times \boldsymbol{\nabla}_\perp B_z\right]. \end{aligned} \tag{5.655}$$

Therefore we only have to find E_z, B_z. Let us see what boundary conditions the fields components satisfy at the conducting surfaces, wehre we certainly have

$$\mathbf{E}_\perp = 0, \quad B_z = 0. \tag{5.656}$$

Due to (5.655), this implies $\boldsymbol{\nabla}_\perp \partial_z E_z|_{\rm surface} = 0$. The Maxwell equations admit two types of standing-wave solutions with these conditions:
1) Transverse magnetic waves

$$\begin{aligned} B_z &\equiv 0, \\ E_z &= \varphi_E(\mathbf{x}_\perp)\cos\frac{\pi z}{d}n \quad\quad n = 0,1,2,\dots\ , \end{aligned} \tag{5.657}$$

2) Transverse electric waves

$$\begin{aligned} E_z &\equiv 0, \\ B_z &= \varphi_B(\mathbf{x}_\perp)\sin\frac{\pi z}{d}n \quad\quad n = 1,2,3,\dots\ , \end{aligned} \tag{5.658}$$

where $\varphi_{E,B}(\mathbf{x}_\perp)$ solve the transverse Helmholtz equation

$$\left(\boldsymbol{\nabla}_\perp{}^2 + \omega^2 - k_z{}^2\right)\varphi_{E,B}(\mathbf{x}_\perp) = 0. \tag{5.659}$$

If the dimensions of the box along x- and y-axes are much larger that d, the quantization of the transverse momenta becomes irrelevant. Any boundary condition will yield a nearly continuous set of states with the transverse density of states $L_xL_y/(2\pi)^2$. Thus we may record that there are two standing waves for each momentum

$$\mathbf{k} = \left(k_x, k_y, k_z^n = \frac{\pi}{d}n\right), \tag{5.660}$$

except for the case $n = 0$ when there is only one wave: the transverse magnetic one. Using the discrete momenta in the sum (5.646), the energy between the plates may therefore be written as

$$E_d = \frac{\hbar c}{2}L_xL_y\int\frac{dk_xdk_y}{(2\pi)^2}2\sum_{k_z^n}{}'\sqrt{k_x^2+k_y^2+k_z^{n\,2}}. \tag{5.661}$$

We have reinserted the proper fundamental constants $\hbar$ and c, for convenience. The sum carries a prime which is supposed to record the presence of an extra factor $\frac{1}{2}$ for $n = 0$. In the two semi-infinite regions outside the two plates also the momentum k_z may be taken as a continuous variable so that there are the additional vacuum energies

$$\begin{aligned} E_{\rm outside} &= \frac{\hbar c}{2}L_xL_y\frac{L_z}{2}\int\frac{dk_xdk_ydk_z}{(2\pi)^3}2\sqrt{k_x^2+k_y^2+k_z^2} \\ &+ \frac{\hbar c}{2}L_xL_y\left(\frac{L_z}{2}-d\right)\int\frac{dk_xdk_ydk_z}{(2\pi)^3}2\sqrt{k_x^2+k_y^2+k_z^2}. \end{aligned} \tag{5.662}$$

Let us now compare this energy with the corresponding expression in the absence of the plates

$$E_0 = \frac{\hbar c}{2} L_x L_y L_z \int \frac{dk_x dk_y dk_z}{(2\pi)^3} 2\sqrt{k_x^2 + k_y^2 + k_z^2}. \tag{5.663}$$

By subtracting this from $E_d + E_{\text{outside}}$ we find the change of the energy due to the presence of the plates

$$\Delta E = \hbar c L_x L_y \int \frac{dk_x dk_y}{(2\pi)^2} \left(\sum_{k_z = k_z^n}{}' - \int_0^\infty \frac{dk_z d}{\pi} \right) \sqrt{k_x^2 + k_y^2 + k_z^2}. \tag{5.664}$$

It is caused by the difference in the particle spectra, once with discrete k_z^n between the plates and once with continuous k_z without plates. The evaluation of (5.664) proceeds in two steps. First we integrate over the $k_\perp = (k_x, k_y)$ variables but enforce the convergence by inserting a *cutoff function* $f(k_\perp^2 + k_z^2)$ which is identical to unity up to some large $\mathbf{k}^2 = k_\perp^2 + k_z^2$, say $\mathbf{k}^2 = \Lambda^2$. For $\mathbf{k}^2 \gg \Lambda^2$, the cutoff function decreases rapidly to zero. Later we shall be able to take $\Lambda^2 \to \infty$. The cutoff function is necessary to perform the mathematical operations. In the physical system a function of this type is provided by the finite thickness and conductivity of the plates. This will have the effect that for wavelengths much smaller than the thickness, the plates become transparent to the electromagnetic waves. Thus they are no longer able to enforce the boundary conditions which are essential for the discreteness of the spectrum. Since the energy difference comes mainly from the long wavelengths, the precise way in which the short wavelengths are cutoff is irrelevant.

We then proceed by considering the remaining function of k_z

$$g(k_z) \equiv \int dk_\perp^2 \sqrt{k_\perp^2 + k_z^2} f(k_\perp^2 + k_z^2), \tag{5.665}$$

in terms of which the energy difference is given by

$$\Delta E = \hbar c L_x L_y \frac{1}{4\pi^2} \left(\sum_{k_z = k_z^n}{}' - \int_0^\infty \frac{dk_z d}{\pi} \right) g(k_z). \tag{5.666}$$

To evaluate this expression it is convenient to change the variables from k_z^n to $n = k_z d/\pi$ and from $k_\perp^2$ to $\nu^2 = k_\perp^2 d^2/\pi^2$, and to introduce the auxiliary function

$$\begin{aligned} G(n) &\equiv \frac{d^3}{\pi^4} g(\pi n/d) = \frac{d^3}{\pi^3} \int_{\pi^2 n^2/d^2}^\infty dk^2\, k f(k^2) \\ &= \int_{n^2}^\infty d\nu^2 \nu f\left(\pi^2 \nu^2/d^2\right). \end{aligned} \tag{5.667}$$

Then ΔE can be written as

$$\Delta E = \hbar c L_x L_y \frac{\pi^2}{4d^3} \left[\sum_{n=0}^{\infty}{}' G(n) - \int_0^\infty dn\, G(n) \right]. \tag{5.668}$$

The difference between a sum and an integral over the function $G(n)$ is given by the well-known Euler-Maclaurin formula which reads [see Eq. (5C.20) in Appendix 5C]

$$\frac{1}{2}G(0) + G(1) + G(2) + \ldots + G(n-1) + \frac{1}{2}G(n) - \int_0^n dn\, G(n) \\ = \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}\left[G^{(2k-1)}(n) - G^{(2k-1)}(0)\right]. \tag{5.669}$$

Here B_k are the Bernoulli numbers, defined by the Taylor expansion [see (5C.15)]

$$\frac{t}{e^t - 1} = \sum_{k=0}^{\infty} B_k \frac{t^k}{k!}, \tag{5.670}$$

whose lowest values are [see (5C.6)]

$$B_0 = 1,\ B_1 = -\frac{1}{2},\ B_2 = \frac{1}{6},\ B_3 = 0,\ B_4 = -\frac{1}{30},\ B_5 = 0,\ B_6 = \frac{1}{42},\ \ldots. \tag{5.671}$$

The primed sum in (5.661) is therefore obtained from the expansion

$$\begin{aligned} \sum_{n=0}^{\infty}{}' G(n) - \int_0^{\infty} dn\, G(n) &= -\frac{B_2}{2!}[G'(0) - G'(\infty)] \\ &\quad -\frac{B_4}{4!}[G'''(0) - G'''(\infty)] \\ &\quad -\frac{B_6}{6!}[G^{(5)}(0) - G^{(5)}(\infty)] \\ &\quad \vdots \end{aligned} \tag{5.672}$$

Since the cutoff function $f(\mathbf{k}^2)$ vanishes exponentially fast at infinity, the function $G(n)$ and all its derivatives vanish in the limit $n \to \infty$ (so that the factor $1/2$ at the upper end of the primed sum is irrelevant) For $n = 0$, only one expansion coefficient turns out to be nonzero. To see this, we denote $f(\pi^2 n^2/d^2)$ by $\tilde{f}(n^2)$ and calculate

$$\begin{aligned} G'(0) &= -[2n^2 \tilde{f}(n^2)]_{n=0} = 0, \\ G''(0) &= -\left[4n\tilde{f}\left(n^2\right) + 4n^3\tilde{f}'\left(n^2\right)\right]_{n=0} = 0, \\ G'''(0) &= -\left[4\tilde{f}\left(n^2\right) + 18n^2\tilde{f}'\left(n^2\right) + 8n^4\tilde{f}''(n^2)\right]_{n=0} = -4, \\ G^{(l)}(0) &= 0, \quad l > 3. \end{aligned} \tag{5.673}$$

The higher derivatives contain an increasing number of derivatives of $\tilde{f}(\nu^2)$. Since $\tilde{f}(\nu^2)$ starts out being unity up to large arguments, all derivatives vanish at $\nu = 0$. Thus we arrive at

$$\sum_{n=0}^{\infty}{}' G(n) - \int_0^{\infty} dn\, G(n) = 4\frac{B_4}{4!} = -\frac{1}{180}. \tag{5.674}$$

This yields the energy difference

$$\Delta E = -L_x L_y \hbar c \frac{\pi^2}{720 d^3}. \tag{5.675}$$

There is an attractive force between silver plates decreasing with the inverse forth power of the distance:

$$F = -L_x L_y \hbar c \frac{\pi^2}{240 d^4}. \tag{5.676}$$

Between steel plates of area 1 cm^2 and distance 0.5 μm, the force is 0.2 dyne/cm^2. The existence of this force was verified experimentally.[30]

In dielectric media, a similar calculation renders the important van der Waals forces between two plates of different dielectric constants.[31]

5.11 ZETA FUNCTION REGULARIZATION

There exists a more elegant method of evaluating the energy difference (5.664) without using a cutoff function $f(\mathbf{k}^2)$. This method has become popular in recent years in the context of the field theories of critical phenomena near second-order phase transitions. The method will be discussed in detail when calculating the properties of interacting particles in Chapter 24. The Casimir effect presents a good opportunity for a short introduction. We observe that we can rewrite an arbitrary negative power of a positive quantity a as an integral

$$a^{-z} = \frac{1}{\Gamma(z)} \int_0^\infty \frac{d\tau}{\tau} \tau^z e^{-\tau a}. \tag{5.677}$$

This follows by a simple rescaling from the integral representation for the Gamma function[32]

$$\Gamma(z) = \int_0^\infty \frac{d\tau}{\tau} \tau^z e^{-\tau}. \tag{5.678}$$

which converges for Re $z > 0$. Then we rewrite the energy difference (5.664) as

$$\Delta E = \hbar c L_x L_y \int \frac{dk_x dk_y}{(2\pi)^2} \left(\sum_{k_z = k_z^n}{}' - \int_0^\infty \frac{dk_z d}{\pi} \right) (k_x^2 + k_y^2 + k_z^2)^{-z}, \tag{5.679}$$

and evaluate this exactly for sufficiently large z, where sum and integrals converge. At the end we continue the result analytically to $z = -1/2$.

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[30] M.J. Sparnay Physica *24*, 751 (1958); J. Tabor and R.H.S. Winterton, Nature *219*, 1120 (1968); T.H. Boyer, Annals of Physics *56*, 474 (1970); S.K. Lamoreaux, Phys. Rev. Lett. *78*, 5 (1997). See also G. Esposito, A.Y. Kamenshchik, K. Kirsten, *On the Zero-Point Energy of a Conducting Spherical Shell*, (hep-th/9707168).

[31] See H. Kleinert, Phys. Lett. A *136*, 253 (1989), and references therein.

[32] I.S. Gradshteyn and I.M. Ryzhik, op. cit., Formula 8.310.1.

If we dont worry about the convergence at each intermediate step, this procedure is equivalent to using formula (5.680) for $z = -1/2$

$$\sqrt{a} = \frac{1}{\Gamma(-1/2)} \int_0^\infty \frac{d\tau}{\tau} \tau^{-1/2} e^{-\tau a}, \tag{5.680}$$

and rewriting the energy difference (5.664) as

$$\Delta E = \hbar c L_x L_y \frac{1}{\Gamma(-1/2)} \int_0^\infty \frac{d\tau}{\tau} \tau^{-1/2} \int \frac{dk_x dk_y}{(2\pi)^2} \left({\sum_{k_z = k_z^n}}' - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau(k_x^2 + k_y^2 + k_z^2)}. \tag{5.681}$$

Being Gaussian, the integrals over k_x, k_y can immediately be done, yielding

$$\Delta E = \hbar c L_x L_y \frac{1}{4\pi\Gamma(-1/2)} \int_0^\infty \frac{d\tau}{\tau} \tau^{-3/2} \left({\sum_{k_z = k_z^n}}' - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2}. \tag{5.682}$$

The remaining sum-minus-integral over k_z is evaluated as follows. First we write

$$\left({\sum_{k_z = k_z^n}}' - \int_0^\infty \frac{dk_z d}{\pi} \right) e^{-\tau k_z^2} = \frac{1}{2} \left(\sum_{n=-\infty}^{\infty} - \int_{-\infty}^{\infty} dn \right) e^{-\tau \pi^2 n^2 / d^2}. \tag{5.683}$$

Then we make use of the *Poisson formula*[33]

$$\sum_{m=-\infty}^{\infty} e^{2\pi i \mu m} = \sum_{n=-\infty}^{\infty} \delta(\mu - n). \tag{5.684}$$

This allows us to express the sum over n as an integral over n, which is restricted to the original sum with the help of an extra sum over integers m:

$$\frac{1}{2} \sum_{n=-\infty}^{\infty} e^{-\alpha n^2} = \frac{1}{2} \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dn \, e^{-\alpha n^2 + 2\pi i n m}. \tag{5.685}$$

The Gaussian integral over n can then be performed after a quadratic completion, and gives

$$\frac{1}{2} \sum_{n=-\infty}^{\infty} e^{-\alpha n^2} = \frac{1}{2} \sum_{m=-\infty}^{\infty} \sqrt{\frac{\pi}{\alpha}} e^{-4\pi^2 m^2 / \alpha}. \tag{5.686}$$

The two sides are said to be the *dual transforms* of each other. The left-hand side converges fast for large α, the right-hand side does so for small α. This duality transformation is fundamental to the theoretical description of many phase transitions where the partition functions over fundamental excitations can be brought to different forms by such transformations, one converging fast for low temperatures, the other for high temperatures.[34]

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[33] For a proof see H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics,* World Scientific., Singapore 1995 (second edition), p. 124.

Now, subtracting from the sum (5B.7) over n the integral over dn removes from the auxiliary sum over m on the right-hand side precisely the $m=0$ term, so that we find the difference between sum and integral:

$$\frac{1}{2}\left(\sum_{n=-\infty}^{\infty}-\int_{-\infty}^{\infty}dn\right)e^{-\alpha n^2}=\sum_{m=1}^{\infty}\sqrt{\frac{\pi}{\alpha}}e^{-4\pi^2m^2/\alpha}. \tag{5.687}$$

The left-hand side appears directly in (5.683), which therefore becomes

$$\left(\sum_{k_z=k_z^n}{}'-\int_0^{\infty}\frac{dk_zd}{\pi}\right)e^{-\tau k_z^2}=\frac{d}{\sqrt{\pi\tau}}\sum_{m=1}^{\infty}e^{-d^2m^2/\tau}. \tag{5.688}$$

To obtain the energy difference (5.682), this has to be multiplied by $\tau^{-3/2}$ and integrated over $d\tau/\tau$. In the dually transformed integral, convergence at small τ is automatic. The τ integral can be done yielding

$$\int_0^{\infty}\frac{d\tau}{\tau}\tau^{-3/2}\frac{d}{\sqrt{\pi\tau}}\sum_{m=1}^{\infty}e^{-d^2m^2/\tau}=\frac{d}{\sqrt{\pi}}\frac{\Gamma(2)}{d^4}\sum_{m=1}^{\infty}\frac{1}{m^4}. \tag{5.689}$$

The sum over m involves Riemann's zeta function

$$\zeta(x)\equiv\sum_{m=1}^{\infty}\frac{1}{m^x}, \tag{5.690}$$

encountered before in statistical mechanics calculations [see (2.276)], and is equal to [recall (2.315)]

$$\zeta(4)=\frac{8\pi^4}{4!}|B_4|=\frac{8\pi^4}{4!}\frac{1}{30}. \tag{5.691}$$

With this number, the energy difference (5.682) becomes, recalling the values of the Gamma function $\Gamma(2)=1$ and $\Gamma(-1/2)=-2\sqrt{\pi}$,

$$\begin{aligned}\Delta E &= \hbar cL_xL_y\frac{1}{4\pi\Gamma(-1/2)}\int_0^{\infty}\frac{d\tau}{\tau}\tau^{-3/2}\left(\sum_{k_z=k_z^n}{}'-\int_0^{\infty}\frac{dk_zd}{\pi}\right)e^{-\tau k_z^2}\\ &= \hbar cL_xL_y\frac{\Gamma(2)}{4\pi^{3/2}\Gamma(-1/2)d^3}=-L_xL_y\hbar c\frac{\pi^2}{720d^3}.\end{aligned} \tag{5.692}$$

This is the same result as in Eq. (5.675). To be completely satisfactory, these calculations should all be done for the general expression (5.679), followed by an analytic continuation of the power z to $-1/2$ at the end.

---

[34] For a comprehensive discussion see the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I *Superflow and Vortex Lines*, pp. 1–744, and Vol. II *Stresses and Defects*, pp. 744-1443, World Scientific Publishing Co., Singapore 1989.

While being formal, with the above justification via analytic continuation, we may be mathematically even more sloppy, and process the τ-integral in the energy difference (5.682) as a shortcut via (5.683) and write

$$\int_0^\infty \frac{d\tau}{\tau}\tau^{-3/2}\left(\sum_{k_z=k_z^n}{}' - \int_0^\infty \frac{dk_z d}{\pi}\right) e^{-\tau k_z^2} = \frac{1}{2}\left(\sum_{n=-\infty}^{\infty} - \int_{-\infty}^{\infty} dn\right)\int_0^\infty \frac{d\tau}{\tau}\tau^{-3/2} e^{-\tau\pi^2 n^2/d^2}$$

$$= \Gamma(-3/2)\left(\sum_{n=-\infty}^{\infty}{}' - \int_0^\infty dn\right) n^3. \qquad (5.693)$$

The divergent sum-minus-integral over n^3 can formally identified with the zeta function $\sum_{n=1}^{\infty} n^{-z}$ at the negative argument $z=-3$. With the help of formula (2.312), we find

$$\zeta(-3) = -\frac{B_4}{4} = \frac{1}{120}. \qquad (5.694)$$

In serting this together $\Gamma(-3/2) = -2\Gamma(-1/2)/3$ into

$$\Delta E = -L_x L_y \hbar c \frac{\pi^2}{720 d^3}. \qquad (5.695)$$

The correctness of this formal approach is ensured by the explicit duality transformation done before.

The formal procedure of evaluating apparently meaningless sum-minus-integrals over powers n^ν with $\nu > -1$ using zeta functions of negative arguments is known as the *zeta function regularization* method.

We shall see later in Eq. (9.126), that by a similar analytic continuation an integral $\int_0^\infty dk\, k^\alpha$ vanishes for all α. For this reason, the zeta-function regularization applies even to the pure sum, allowing us to replace $\sum_{n=1}^{\infty} n^\nu$ by $\zeta(\nu)$.

5.12 FREE GREEN FUNCTIONS OF n FIELDS

For free fields of spin 0 and 1/2 quantized in the preceding sections we have shown that the vacuum expectation value of the time-ordered product of two field operators, the propagator, is equal to the Green function associated with the differential equation obeyed by the field. In the case of the real Klein-Gordon field we had, for example,

$$G(x_1, x_2) = G(x_1 - x_2) \equiv \langle 0|T\phi(x_1)\phi(x_2)|0\rangle \qquad (5.696)$$

satisfying

$$(-\partial^2 - M^2)G(x, x_2) = i\delta^{(4)}(x - x_2). \qquad (5.697)$$

It is useful to define a generalization of the vacuum expectation values (5.696) to any number n of free fields:

$$G^{(n)}(x_1, x_2, x_3, \dots, x_n) \equiv \langle 0|T\phi(x_1)\dots\phi(x_n)|0\rangle. \qquad (5.698)$$

This object will be referred to as the free *n-point propagator* or *n-point function*, or *n-point Green function*[35] For complex scalar fields, the appropriate definition is

$$G^{(n,m)}(x_1,\dots,x_n;x'_1,\dots,x'_m) \equiv \langle 0|T\phi(x_1)\cdots\phi(x_n)\phi^\dagger(x'_1)\cdots\phi^\dagger(x'_m)|0\rangle. \tag{5.699}$$

For free fields, the latter is nonzero only for $n = m$. Corresponding expressions are used for fields of any spin. We shall see later that the set of all free n-point functions plays a crucial role in extracting the information contained in an arbitrary interacting field theory.

The n-point functions may be considered as the relativistic generalizations of the set of all many-particle Schrödinger wave functions in the nonrelativistic theory. In the local $\mathbf{x}$-basis, these would consist in the set of all scalar products

$$\langle \mathbf{x}_1,\dots,\mathbf{x}_n|\psi(t)\rangle = \langle 0|\psi(\mathbf{x}_1,0)\cdots\psi(\mathbf{x}_n,0)|\psi(t)\rangle. \tag{5.700}$$

Choosing for the wave vectors $|\psi(t)\rangle$ any state in the local n-particle basis

$$|\mathbf{x}'_1,\dots,\mathbf{x}'_n;t\rangle = \psi^\dagger(\mathbf{x}'_1,t)\cdots\psi^\dagger(\mathbf{x}'_n,t)|0\rangle, \tag{5.701}$$

we arrive at the scalar products

$$\langle 0|\psi(\mathbf{x},0)\cdots\psi(\mathbf{x}_n,0)\psi^\dagger(\mathbf{x}'_1,t)\cdots\psi^\dagger(\mathbf{x}'_n,t)|0\rangle. \tag{5.702}$$

These, in turn, are a special sort of propagator,

$$G^{(n,m)}(\mathbf{x}_1,0,\mathbf{x}_2,0,\dots,\mathbf{x}_n,0;\mathbf{x}'_1,t,\dots,\mathbf{x}'_m,t), \tag{5.703}$$

where only two time arguments appear. When going to relativistic theories, the set of such equal-time objects is no longer invariant under Lorentz transformations. Two events which happen simultaneously in one frame do not in another frame. This is why the propagators $G^{(n,m)}(x,\dots,x_n;x'_1,\dots,x'_m)$ with arbitrary spacetime arguments represent the relativistic generalization of the local wave functions. This argument does not yet justify the time ordering in the relativistic propagators in contrast to the relevance of the causal propagator in the nonrelativistic case. Its advantage will become apparent only later in the development of perturbation theory.

At the present level where we are dealing only with free quantum fields, the n-point functions are not really independent objects. They can all be expanded into a sum of products of the simple propagators. Before we develop the main expansion formula it is useful to recall the definition of a normal product introduced in Subsecs. 5.1.5 and 5.3.2 for Bose and Fermi fields, respectively. There it was contrived as a trick to eliminate a bothersome infinite energy of the vacuum to the zero-point oscillations of the free fields, to circumvent a proper physical discussion. Here we need this product for purely mathematical reasons to help us evaluating vacuum expectation values of products of many field operators.

---

[35] For massive vector fields and other massive fields with spin larger than 1/2, one must watch out for the discrepancy between propagator and Green function by Schwinger terms. For scalar fields, there is no problem of this kind.

Given an arbitrary set of n free field operators $\phi_1(x_1)\cdots\phi_n(x_n)$, each of them consists of a creation and an annihilation part:

$$\phi_i(x_i) = \phi_i^c(x_i) + \phi_i^a(x_i). \tag{5.704}$$

Some ϕ_i may be commuting Bose fields, some anticommuting Fermi fields. The normally ordered product or *normal product* of n of these field operators will be denoted by $N((\phi_1(x)\phi(x_2) \cdots \phi(x_n))$. In the present context, a function symbol will be more convenient than the earlier double-dot notation. The normal product is a function of a product of field operators which has the following two properties:

i) **Linearity**: The normal product is a linear function of all its n arguments, i.e., it satisfies

$$N\left((\alpha\phi_1 + \beta\phi_1')\phi_2\phi_3\cdots\phi_n\right) = \alpha N(\phi_1\phi_2\phi_3\cdots\phi_n) + \beta N(\phi_1'\phi_2\phi_3\cdots\phi_n) \tag{5.705}$$

If every ϕ_i is replaced by $\phi_i^c + \phi_i^a$, it can be expanded into a linear combination of terms which are all pure products of creation and annihilation operators.

ii) **Normal Reordering**: The normal product reorders all products arising from a complete linear expansion of all fields according to i) in such a way that all annihilators stand to the right of all creators. If the operators ϕ_i describe fermions, the definition requires a factor -1 to be inserted for every transmutation of the order of two operators.

For example, let ϕ_1, ϕ_2, ϕ_3 be scalar fields, then normal ordering produces for two field operators

$$\begin{aligned} N(\phi_1^c\phi_2^c) &= \phi_1^c\phi_2^c = \phi_2^c\phi_1^c, \\ N(\phi_1^c\phi_2^a) &= \phi_1^c\phi_2^a, \\ N(\phi_1^a\phi_2^c) &= \phi_2^c\phi_1^a, \\ N(\phi_1^a\phi_2^a) &= \phi_1^a\phi_2^a = \phi_2^a\phi_1^a, \end{aligned} \tag{5.706}$$

and for three field operators

$$\begin{aligned} N(\phi_1^c\phi_2^c\phi_3^a) &= \phi_1^c\phi_2^c\phi_3^a = \phi_2^c\phi_1^c\phi_3^a, \\ N(\phi_1^c\phi_2^a\phi_3^c) &= \phi_1^c\phi_3^c\phi_2^a = \phi_3^c\phi_1^c\phi_2^a, \\ N(\phi_1^a\phi_2^c\phi_3^c) &= \phi_2^c\phi_3^c\phi_1^a = \phi_3^c\phi_2^c\phi_1^a. \end{aligned} \tag{5.707}$$

If the operators ϕ_i are fermions, the effect is

$$\begin{aligned} N(\phi_1^c\phi_2^c) &= \phi_1^c\phi_2^c = -\phi_2^c\phi_1^c, \\ N(\phi_1^c\phi_2^a) &\equiv \phi_1^c\phi_2^a, \\ N(\phi_1^a\phi_2^c) &= -\phi_2^c\phi_1^a, \\ N(\phi_1^a\phi_2^a) &= \phi_1^a\phi_2^a = -\phi_2^a\phi_1^a, \end{aligned} \tag{5.708}$$

and

$$
\begin{aligned}
N(\phi_1^c\phi_2^c\phi_3^a) &= \phi_1^c\phi_2^c\phi_3^a = -\phi_2^c\phi_1^c\phi_3^a, \\
N(\phi_1^c\phi_2^a\phi_3^c) &= -\phi_1^c\phi_3^c\phi_2^a = \phi_3^c\phi_1^c\phi_2^a, \\
N(\phi_1^a\phi_2^c\phi_3^c) &= \phi_2^c\phi_3^c\phi_1^a = -\phi_3^c\phi_2^c\phi_1^a.
\end{aligned} \tag{5.709}
$$

The normal product is uniquely defined. The remaining order of creation or annihilation parts among themselves is irrelevant, since these commute or anticommute with each other by virtue of the canonical free-field commutation rules. In the following, the fields ϕ may be Bose or Fermi fields and the sign of the Fermi case will be recorded underneath the Bose sign.

The advantage of defining normal products is their important property that they have no vacuum expectation values. There is always an annihilator on the right-hand side or a creator on the left-hand side which produce 0 when matched between vacuum states. The method of calculating all n-point functions will consist in expanding all time ordered products of n field operators completely into normal products. Then only the terms with no operators will survive between vacuum states. This will be the desired value of the n-point function.

Let us see how this works for the simplest case of a time-ordered product of two identical field operators

$$
T(\phi(x_1)\phi(x_2)) \equiv \Theta(x_1^0 - x_2^0)\phi(x_1)\phi(x_2) \pm \Theta(x_2^0 - x_1^0)\phi(x_2)\phi(x_1). \tag{5.710}
$$

The basic expansion formula is

$$
T(\phi(x_1)\phi(x_2)) = N(\phi(x_1)\phi(x_2)) + \langle 0|T(\phi(x_1)\phi(x_2))|0\rangle. \tag{5.711}
$$

For brevity, we shall denote the propagator of two fields as follows:

$$
\langle 0|T(\phi(x_1)\phi(x_2))|0\rangle \equiv \dot{\phi}(x_1)\dot{\phi}(x_2) = G(x_1 - x_2). \tag{5.712}
$$

The two dots which mentally connect the two fields are referred to as a *contraction* of the fields.

We shall prove the basic expansion formula (5.711) by considering it separately for the creation and annihilation parts ϕ^c and ϕ^a. This will be sufficient since the time ordered product is linear in each field just as the normal product. Now, in both cases $x_1^0 \gtrless x_2^0$ we have

$$
\begin{aligned}
T(\phi^c(x_1)\phi^c(x_2)) &= \left\{ \begin{array}{c} \phi^c(x_1)\phi^c(x_2) \\ \pm\, \phi^c(x_2)\phi^c(x_1) \end{array} \right\} \\
&= \phi^c(x_1)\phi^c(x_2) + \langle 0| \left\{ \begin{array}{c} \phi^c(x_1)\phi^c(x_2) \\ \pm\, \phi^c(x_2)\phi^c(x_1) \end{array} \right\} |0\rangle,
\end{aligned} \tag{5.713}
$$

which is true since $\phi^c(x_1)\phi^c(x_2)$ commute or anticommute with each other, and annihilate the vacuum state $|0\rangle$. The same equation holds for $\phi^a(x_1)\phi^a(x_2)$. The only nontrivial cases are those with a time-ordered product of $\phi^c(x_1)\phi^a(x_2)$ and $\phi^a(x_1)\phi^c(x_2)$. The first becomes for $x_1^0 \gtrless x_2^0$:

$$\begin{aligned} T(\phi^c(x_1)\phi^a(x_2)) &= \left\{ \begin{array}{c} \phi^c(x_1)\phi^a(x_2) \\ \pm\, \phi^a(x_2)\phi^c(x_1) \end{array} \right\} \\ &= \phi^c(x_1)\phi^a(x_2) + \langle 0| \left\{ \begin{array}{c} \phi^c(x_1)\phi^a(x_2) \\ \pm\, \phi^a(x_2)\phi^c(x_1) \end{array} \right\} |0\rangle. \end{aligned} \tag{5.714}$$

For $x_1^0 > x_2^0$, this equation is obviously true. For $x_1^0 < x_2^0$, the normal ordering produces an additional term

$$\pm\, (\phi^a(x_2)\phi^c(x_1) \mp \phi^c(x_1)\phi^a(x_2)) = \pm[\phi^a(x_2), \phi^c(x_1)]_{\mp}. \tag{5.715}$$

As the commutator or anticommutator of free fields is a c-number, they may equally well be evaluated between vacuum states, so that we may replace (5.715) by

$$\pm\, \langle 0|\, [\phi^a(x_2), \phi^c(x_1)]_{\mp}\, |0\rangle. \tag{5.716}$$

Moreover, since ϕ^a annihilates the vacuum, this reduces to

$$\pm\, \langle 0|\phi^a(x_2), \phi^c(x_1)|0\rangle. \tag{5.717}$$

The oppositely ordered operators $\phi^a(x_1)\phi^c(x_2)$ can be processed by complete analogy.

We shall now generalize this basic result to an arbitrary number of field operators. In order to abbreviate the expressions let us define the concept of a contraction inside a normal product

$$\begin{aligned} &N\left(\phi_1 \cdots \phi_{i-1}\dot{\phi}_i\phi_{i+1} \cdots \phi_{j-1}\dot{\phi}_j\phi_{j+1} \cdots \phi_n\right) \\ &\qquad \equiv \eta\dot{\phi}_i\dot{\phi}_j N\left(\phi_1 \cdots \phi_{i-1}\phi_{i+1} \cdots \phi_{j-1}\phi_{j+1} \cdots \phi_n\right). \end{aligned} \tag{5.718}$$

Here $\eta = 1$ for bosons and $(-1)^{j-i-1}$ for fermions accounting for the number of fermion transmutations necessary to reach the final order. A normal product with several contractions is defined by the successive execution of each of them. If only one field is left inside the normal ordering symbol it is automatically normally ordered so that

$$N(\phi) = \phi. \tag{5.719}$$

Similarly, if all fields inside a normal product are contracted, the result is no longer an operator and the symbol N may be dropped using linearity and the trivial property

$$N(1) \equiv 1. \tag{5.720}$$

The fully contracted normal product will be the relevant one in determining the n-particle propagator. With these preliminaries we are now ready to prove *Wick's theorem* for the expansion of a time-ordered product in terms of normally ordered products.[36]

---

[36] G.C. Wick, Phys. Rev. *80*, 268 (1950); F. Dyson, Phys. Rev. *82*, 428 (1951).

5.12.1 Wick's Theorem

The theorem may be stated as follows. An arbitrary time ordered product of free fields can be expanded into a sum of normal products one for each different contraction between pairs of operators:

$$\begin{aligned}
&T(\phi_1\cdots\phi_n) = N(\phi_1\cdots\phi_n) \qquad \text{(no contraction)}\\
&+N(\dot\phi_1\dot\phi_2\phi_3\cdots\phi_n)+N(\dot\phi_1\phi_2\dot\phi_3\cdots\phi_n)+\ldots+N(\dot\phi_1\phi_2\phi_3\cdots\dot\phi_n)\\
&+N(\phi_1\dot\phi_2\dot\phi_3\cdots\phi_n)+\ldots+N(\phi_1\dot\phi_2\cdots\dot\phi_n)+\ldots \quad \text{(one contraction)}\\
&+N(\dot\phi_1\dot\phi_2\ddot\phi_3\ddot\phi_4\phi_5\cdots\phi_n)+N(\dot\phi_1\dot\phi_2\ddot\phi_3\phi_4\ddot\phi_5\cdots\phi_n)\\
&+N(\dot\phi_1\ddot\phi_2\dot\phi_3\ddot\phi_4\phi_5\cdots\phi_n)+N(\dot\phi_1\ddot\phi_2\dot\phi_3\phi_4\ddot\phi_5\cdots\phi_n)+\ldots \quad \text{(two contractions)}\\
&+\ldots\\
&+N(\dot\phi_1\dot\phi_2\ddot\phi_3\ddot\phi_4\dddot\phi_5\dddot\phi_6\cdots\ddddot\phi_{n-1}\ddddot\phi_n)+N(\dot\phi_1\ddot\phi_2\dot\phi_3\ddot\phi_4\dddot\phi_5\dddot\phi_6\cdots\ddddot\phi_{n-1}\ddddot\phi_n)\\
&+\ldots \qquad \text{(all contractions).} \qquad\qquad (5.721)
\end{aligned}$$

In this particular expression we have assumed n to be even so that it is possible to contract all operators. Otherwise each term in the last row would have contained one uncontracted field. In either case the expansion on the right-hand side will be abbreviated as

$$\sum_{\text{all pair contractions}} N(\phi_1\cdots\phi_n), \qquad (5.722)$$

i.e., we shall state Wick's theorem in the form

$$T(\phi_1\cdots\phi_n) = \sum_{\text{all pair contractions}} N(\phi_1\cdots\phi_n). \qquad (5.723)$$

Using Wick's theorem it is a trivial matter to calculate an arbitrary n-point function of free fields. Since the vacuum expectation values of all normal products are zero except for the fully contracted ones we may immediately write for an even number of real fields:

$$\begin{aligned}
G^{(n)}(x_1\cdots x_n) &= \langle 0|T\left(\phi(x_1)\cdots\phi(x_n)\right)|0\rangle\rangle\\
&= \sum_{\text{all full pair contractions}} N\left(\phi(x_1)\cdots\phi(x_n)\right). \qquad (5.724)
\end{aligned}$$

A simple combinatorical analysis shows that the right-hand side consists of

$$n!/(n/2)!2^{n/2} = 1\cdot 3\cdot 5\cdots(n-1)\equiv(n-1)!!$$

pair terms.

In the case of complex fields, $G^{(n,m)}$ can only be nonzero for $n=m$ and all contractions $\dot\phi\dot\phi$ and $\dot\phi^\dagger\dot\phi^\dagger$ vanish. Thus there are altogether $n!$ different contractions.

The proof of (5.723) goes by induction: For $n=2$ the theorem was proved in Eq. (5.711). Let it be true for a product of n fields $\phi_1\cdots\phi_n$, and allow for an additional field ϕ. We may assume that it is earlier in time than the other fields

$\phi_1, \ldots, \phi_n$. For if it were not, we could always choose the earliest of the n fields, move it completely to the right in the time ordered product, with a well-defined phase factor due to Femi permutations, and proceed as we shall now do. Once the rightmost field is the earliest, it may be removed trivially from the time ordered product. The resulting product can be expanded according to the Wick's theorem for a product of n field operators as

$$T(\phi_1 \cdots \phi_n \phi) = T(\phi_1 \cdots \phi_n)\phi = \sum_{\text{all pair contractions}} N(\phi_1 \cdots \phi_n)\phi. \tag{5.725}$$

We now incorporate the extra field ϕ on the right-hand side into each of the normal product in the expansion. When doing so we obtain from each term precisely the contractions required by Wick's theorem for $n+1$ field operators. The crucial formula which yields these is

$$\begin{aligned} N(\phi_1 \cdots \phi_n)\phi = {} & N(\phi_1 \cdots \phi_n \phi) + N(\phi_1 \cdots \dot{\phi}_n \dot{\phi}) + N(\phi_1 \cdots \dot{\phi}_{n-1} \phi_n \dot{\phi}) + \ldots \\ & + N(\phi_1 \dot{\phi}_2 \cdots \phi_n \dot{\phi}) + N(\dot{\phi}_1 \phi_2 \cdots \phi_n \dot{\phi}), \end{aligned} \tag{5.726}$$

which is valid as long as ϕ is earlier than the others. This formula is proved by splitting ϕ into creation and annihilation parts and considering each part separately, which is allowed because of the linearity of the normal products. For $\phi = \phi^a$, the formula is trivially true since all contractions vanish. Indeed, for a field ϕ^a with an earlier time arguments than that of all others, we find:

$$\dot{\phi}_i \dot{\phi}^a \equiv \langle 0|T(\phi(x_i)\phi^a(x))|0\rangle = \langle 0|\phi(x_i)\phi^a(x)|0\rangle \equiv 0. \tag{5.727}$$

For $\phi = \phi^c$, let us for a moment assume that all other ϕ_i's are annihilating parts ϕ_i^a. If one or more creation parts ϕ_i^c are present, they will appear as left-hand factors in each normally ordered term of (5.726) and participate only as spectators in the further operations. Thus we prove

$$N(\phi_1^a \cdots \phi_n^a)\phi^c = N(\phi_1^a \cdots \phi_n^a \phi^c) + N(\phi_1^a \cdots \dot{\phi}_n^a \dot{\phi}^c) + \ldots + N(\dot{\phi}_1^a \cdots \phi_n^a \dot{\phi}^c), \tag{5.728}$$

for any ϕ^c earlier than the ϕ_i^a's. This expansion is proved by induction. To start we show that it is true for $n = 2$:

$$N(\phi^a)\phi^c = N(\phi^a \phi^c) + N(\dot{\phi}^a \dot{\phi}^c). \tag{5.729}$$

Using (5.719), the left-hand side is equal to $\phi^a \phi^c$, which can be rewritten as

$$\phi^a \phi^c = \pm \phi^c \phi^a [\phi^a, \phi^c]_{\mp}. \tag{5.730}$$

Since the commutator or anticommutator is a c-number, it can be replaced as in (5.716) by its vacuum expectation value, and thus by a contraction (5.727):

$$[\phi^a, \phi^c]_{\mp} = \langle 0|[\phi^a, \phi^c]_{\mp}|0\rangle = \dot{\phi}^a \dot{\phi}^c. \tag{5.731}$$

Rewriting $\pm \phi^c \phi^a$ as $N(\phi^a \phi^c)$ and trivially as $\dot{\phi}^a \dot{\phi}^c$, we see that (5.729) is true.

Now suppose (5.728) to be true for n factors and consider one more annihilation factor ϕ_0^a inside a normal product. This can immediately be taken outside:

$$N(\phi_0^a\phi_1^a\cdots\phi_n^a)\phi^c = \phi_0^a N(\phi_1^a\cdots\phi_n^a)\phi^c. \tag{5.732}$$

The remainder can be expanded via (5.728):

$$\begin{aligned} N(\phi_0^a\phi_1^a\cdots\phi_n^a)\phi^c \;=\;& \phi_0^a[N(\phi_1^a\cdots\phi_n^a\phi^c)+N(\phi_1^a\cdots\dot{\phi}_n^a\dot{\phi}^c) \\ &+N(\phi_1^a\cdots\dot{\phi}_{n-1}^a\phi_n^a\dot{\phi}_c)+\ldots+N(\dot{\phi}_1^a\phi_2^a\cdots\phi_n^a\dot{\phi}^c)]. \end{aligned} \tag{5.733}$$

The additional ϕ_0^a can now be taken into all the terms where the creation operator ϕ^c appears in a contraction:

$$\begin{aligned} N(\phi_0^a\phi_1^a\cdots\phi_n^a)\phi^c \;=\;& \phi_0^a N(\phi_1^a\cdots\phi_n^a\phi^c)+N(\phi_0^a\phi_1^a\cdots\dot{\phi}_n^a\dot{\phi}^c) \\ &+N(\phi_0^a\phi_1^a\cdots\dot{\phi}_{n-1}^a\phi_n^a\dot{\phi}_c)+\ldots+N(\phi_0^a\dot{\phi}_1^a\phi_2^a\cdots\phi_n^a\dot{\phi}^c). \end{aligned} \tag{5.734}$$

Only in the first term, work is needed to reorder the uncontracted creation operator. Writing out the normal product explicitly this term reads

$$\eta\phi_0^a\phi^c\phi_1^a\cdots\phi_n^a, \tag{5.735}$$

where η denotes the number of fermion transmutations necessary to bring ϕ^c from the right-hand side to its normal position. This product can now be rewritten in normal form by using one additional commutator or anticommutator:

$$\pm\,\eta\phi^c\phi_0^a\phi_1^a\cdots\phi_n^a+\eta[\phi_0^a,\phi^c]_\mp\phi_1^a\cdots\phi_n^a. \tag{5.736}$$

But the commutator or anticommutator is again a c-number, and since ϕ^c is earlier than ϕ_0^a, it is equal to the contraction $\dot{\phi}_0^a\dot{\phi}^c$. The two terms in (5.736) can therefore be rewritten as normal products

$$N(\phi_0^a\cdots\phi_n^a\phi^c)+N(\dot{\phi}_0^a\cdots\phi_n^a\dot{\phi}^c). \tag{5.737}$$

In both terms we have brought the field ϕ^c back to its original position thereby canceling the sign factors η and $\pm\eta$ in (5.736). These two are just the missing terms in (5.733) to verify the expansion (5.728) for $n+1$ operators, and thus Wick's theorem (5.723).

Examples are

$$T(\phi_1\phi_2\phi_3)=N(\phi_1\phi_2\phi_3)+\dot{\phi}_1\dot{\phi}_2N(\phi_3)\pm\dot{\phi}_1\dot{\phi}_3N(\phi_2)+\dot{\phi}_2\dot{\phi}_3N(\phi_1), \tag{5.738}$$

and

$$\begin{aligned} T(\phi_1\phi_2\phi_3\phi_4) =\;& N(\phi_1\phi_2\phi_3\phi_4) \\ &+\dot{\phi}_1\dot{\phi}_2N(\phi_3\phi_4)\pm\dot{\phi}_1\dot{\phi}_3N(\phi_2\phi_4)+\dot{\phi}_1\dot{\phi}_4N(\phi_2\phi_3) \\ &+\dot{\phi}_2\dot{\phi}_3N(\phi_1\phi_4)\pm\dot{\phi}_2\dot{\phi}_4N(\phi_1\phi_3)+\dot{\phi}_3\dot{\phi}_4N(\phi_1\phi_2) \\ &+\dot{\phi}_1\dot{\phi}_2\ddot{\phi}_3\ddot{\phi}_4\pm\dot{\phi}_1\dot{\phi}_3\ddot{\phi}_2\ddot{\phi}_4+\dot{\phi}_1\dot{\phi}_4\ddot{\phi}_2\ddot{\phi}_3. \end{aligned} \tag{5.739}$$

Each expansion contains $(n-1)!!$ fully contracted terms.

There is a useful lemma to Wick's theorem which helps in evaluating vacuum expectation values of ordinary products of field operators rather than time-ordered ones. An ordinary product can be expanded in a sum of normal products with all possible pair contractions just as in (5.721), except that contractions stand for commutators of the creation and annihilation parts of the fields, which are c-numbers:

$$\dot{\phi}(x_1)\dot{\phi}(x_2) \equiv [\phi^a(x_1), \phi^c(x_2)]. \tag{5.740}$$

The proof proceeds by induction in the same way as before except that one does not have to make the assumption of the additional field ϕ in the induction is the earliest of all field operators. For the calculation of scattering amplitudes we shall need both expansions.

5.13 Functional Form of Wick's Theorem

Although Wick's rule for expanding the time ordered product of n fields in terms of normal products is quite transparent, it is somewhat cumbersome to state explicitly for any n, as we can see in formula (5.721). It would be useful to find an algorithm which specifies the expansion compactly in mathematical terms. This would greatly simplify further manipulations of operator products. Such an algorithm can easily be found. Let $\delta/\delta\phi(x)$ denote the functional differentiations for functions of space and time, i.e.,

$$\frac{\delta\phi(x)}{\delta\phi(x')} = \delta^{(4)}(x-x'). \tag{5.741}$$

Then we see immediately that the basic formula (5.711) can be rewritten

$$T(\phi(x_1)\phi(x_2)) = \left(1 \pm \frac{1}{2}\int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)} G(y_1,y_2) \frac{\delta}{\delta\phi(y_2)}\right) N(\phi(x_1)\phi(x_2)). \tag{5.742}$$

where functional differentiation treats field variables as c-numbers. The differentiation produces the single possible contraction which by (5.712) is equal to the free propagator $G(x_1,x_2)$. For three operators, the Wick expansion

$$\begin{aligned} T(\phi(x_1)\phi(x_2)\phi(x_3)) &= N(\phi(x_1)\phi(x_2)\phi(x_3)) + N(\dot{\phi}(x_1)\dot{\phi}(x_2)\phi(x_3)) \\ &+ \; N(\dot{\phi}(x_1)\phi(x_2)\dot{\phi}(x_3)) + N(\phi(x_1)\dot{\phi}(x_2)\dot{\phi}(x_3)) \end{aligned} \tag{5.743}$$

can once more be obtained via the same operation

$$\left(1 \pm \frac{1}{2}\int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)} G(y_1,y_2) \frac{\delta}{\delta\phi(y_2)}\right) N(\phi(x_1)\phi(x_2)\phi(x_3)). \tag{5.744}$$

If we want to recover the correct signs for fermions we have to imagine the differentiation variables $\phi(x)$ to be anticommuting objects, $\phi(x)\phi(y) = -\phi(y)\phi(x)$, and use the rule $G(x_1,x_2) = -G(x_2,x_1)$ for fermions.

A time-ordered product of four field operators has a Wick expansion

$$\begin{aligned} T(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) &= N(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) \\ &+ \sum_{\text{one pair contractions}} N(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) \\ &+ \sum_{\text{two pair contractions}} N(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)). \end{aligned} \tag{5.745}$$

Here we can obtain the same result by applying the functional differentiation

$$\begin{aligned} \bigg\{1 \pm \frac{1}{2}\int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)}G(y_1,y_2)\frac{\delta}{\delta\phi(y_2)} \\ +\frac{1}{8}\left(\int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)}G(y_1,y_2)\frac{\delta}{\delta\phi(y_2)}\right)^2\bigg\}. \end{aligned} \tag{5.746}$$

This looks like the first three pieces of a Taylor expansion of the exponential

$$\exp\left\{\pm\frac{1}{2}\int d^4y_1 d^4y_2 \frac{\delta}{\delta\phi(y_1)}G(y_1,y_2)\frac{\delta}{\delta\phi(y_2)}\right\}.$$

Indeed, we shall now prove that the general Wick expansion is given by the functional formula

$$T(\phi(x_1)\cdots\phi(x_n)) = e^{\pm\frac{1}{2}\int d^4y_1 \int d^4y_2 \frac{\delta}{\delta\phi(y_1)}G(y_1,y_2)\frac{\delta}{\delta\phi(y_2)}} N(\phi(x_1)\cdots\phi(x_n)). \tag{5.747}$$

To prepare the tools for deriving this result we introduce the following generating functionals of ordinary, time-ordered, and normal-ordered operator products, respectively:

$$\begin{aligned} O[j] &\equiv e^{i\int d^4x\, j(x)\phi(x)}, \\ T[j] &\equiv Te^{i\int d^4x\, j(x)\phi(x)}, \\ N[j] &\equiv Ne^{i\int d^4x\, j(x)\phi(x)}. \end{aligned} \tag{5.748}$$

Here $j(x)$ is an arbitrary c-number local source term, usually referred to as an *external current*. For Fermi fields $\phi(x)$, the currents have to be anticommuting Grassmann variables which also anticommute with the fields. Under complex conjugation, products of Grassmann variables interchange their order. The product $j(x)\phi(x)$ has therefore the complex-conjugation property

$$[j(x)\phi(x)]^* = -\phi(x)j(x). \tag{5.749}$$

Expressions (5.748) are operators and have the obvious property that their nth functional derivatives with respect to $j(x)$ evaluated at $j(x) \equiv 0$ give the corresponding operator products of n fields:

$$\phi(x_1)\cdots\phi(x_n) = (-i)^n \frac{\delta}{\delta j(x_1)}\cdots\frac{\delta}{\delta j(x_n)}O[j]\bigg|_{j(x)\equiv 0}, \tag{5.750}$$

$$T(\phi(x_1)\cdots\phi(x_n)) = (-i)^n \frac{\delta}{\delta j(x_1)}\cdots\frac{\delta}{\delta j(x_n)}T[j]\bigg|_{j(x)\equiv 0}, \quad (5.751)$$

$$N(\phi(x_1)\cdots\phi(x_n)) = (-i)^n \frac{\delta}{\delta j(x_1)}\cdots\frac{\delta}{\delta j(x_n)}N[j]\bigg|_{j(x)\equiv 0}. \quad (5.752)$$

We can now easily prove Wick's lemma for ordinary products of field operators. We simply separate the field in the generating functional $O[j]$ into creation and annihilation parts:

$$O[j] \equiv e^{i\int d^4x\, j(x)[\phi^a(x)+\phi^c(x)]}, \quad (5.753)$$

and apply the Baker-Hausdorff formula (3.70) to this expression, with $A \equiv i\int d^4x\, j(x)\phi^a(x)$ and $B \equiv i\int d^4x\, j(x)\phi(x)^c$. Because of the anticommutativity of $\phi(x)$ and $j(x)$ for fermions, the commutator $[A,B]$ is

$$[A,B] = -\int d^4x_1 \int d^4x_2\, [\phi^a(x_1),\phi^c(x_2)]_\mp j(x_1)j(x_2), \quad (5.754)$$

and is a c-number. Thus the expansion on the right-hand side of (3.70) terminates, and we can use the formula as

$$e^{A+B} = e^{-\frac{1}{2}[A,B]}e^Ae^B. \quad (5.755)$$

This yields the simple result

$$O[j] = \exp\left\{\frac{1}{2}\int d^4x_1\int d^4x_2\, [\phi^a(x_1),\phi^c(x_2)]_\mp j(x_1)j(x_2)\right\} \\ \times e^{i\int d^4x\, j(x)\phi^c(x)}e^{i\int d^4x\, j(x)\phi^a(x)}. \quad (5.756)$$

The operator on the right-hand side of the curly bracket is recognized to be precisely the generating functional of the normal products:

$$N[j] = e^{i\int d^4x\, j(x)\phi^c(x)}e^{i\int d^4x\, j(x)\phi^a(x)}. \quad (5.757)$$

Now we observe that the currents $j(x)$ in front of this operator are equivalent to a functional differentiation with respect to the fields, $j(x)\hat{=}-i\delta/\delta\phi(x)$. Wick's lemma can therefore be rewritten in the following concise functional form

$$O[j] = \exp\left\{\mp\frac{1}{2}\int d^4x_1\int d^4x_2[\phi^a(x_1),\phi^c(x_2)]_\mp \frac{\delta}{\delta\phi(x_1)}\frac{\delta}{\delta\phi(x_2)}\right\}N[j].$$

The ±-sign appears when commuting or anticommutating $\delta/\delta\phi(x)$ with $j(x)$.

A Taylor expansion of the exponential prefactor renders via the functional derivatives precisely all pair contractions required by Wick's lemma, where a contraction represent a commutator or anticommutator of the fields.

From the earlier proof in Section (5.12.1) it is now clear that exactly the same set of pair contractions appears in the Wick expansion of the time-ordered products of field operators, except that the pair contractions become free-field propagators

$$G(x_1,x_2) \equiv \langle 0|T\left(\phi(x_1)\phi(x_2)\right)|0\rangle. \quad (5.758)$$

Thus we may immediately conclude that Wick's theorem has the functional form

$$T[j] = \exp\left\{\pm\frac{1}{2}\int d^4x_1\int d^4x_2\, G(x_1,x_2)\frac{\delta}{\delta\phi(x_1)}\frac{\delta}{\delta\phi(x_2)}\right\}N[j], \tag{5.759}$$

which becomes, after reexpressing the functional derivatives in terms of the currents,

$$T[j] = e^{-\frac{1}{2}\int d^4y_1 d^4y_2 j(y_1)G(y_1,y_2)j(y_2)}N[j]. \tag{5.760}$$

Expanding both sides in powers of $j(x)$, a comparison of the coefficients yields Wick's expansion for products of any number of time-ordered operators.

The functional $T[j]$ has the important property that its vacuum expectation value

$$Z[j] \equiv \langle 0|T[j]|0\rangle \tag{5.761}$$

collects all informations on n-point functions. Indeed, forming the nth functional derivative as in (5.751) we see that

$$G^{(n)}(x_1,\dots,x_n) = (-i)^n\frac{\delta}{\delta j(x_1)}\cdots\frac{\delta}{\delta j(x_n)}Z[j]. \tag{5.762}$$

For this reason, the vacuum expectation value $Z[j]$ is called the *generating functional* of all n-poin functions. We can take advantage of Wick's expansion formula and write down a compact formula for all n-point functions of free fields. We only have to observe that the generating functional of normal products $N[j]$ has a trivial vacuum expectation value

$$\langle 0|N[j]|0\rangle \equiv 1. \tag{5.763}$$

Then (5.760) leads directly to the simple expression

$$Z[j] = e^{-\frac{1}{2}\int d^4y_1 d^4y_2 j(y_1)G(y_1,y_2)j(y_2)}. \tag{5.764}$$

Expanding the right-hand side in powers of $j(x)$, each term consists of a sum of combinations of propagators $G(x_i,x_{i+1})$. These are precisely the fully pair contracted terms appearing in the Wick expansions (5.724) for the n-point functions

There exists another way of proving Eq. (5.764), by making use of the equation of motion for the field $\phi(x)$. For simplicity, we shall consider a Klein-Gordon field satisfying equation of motion

$$(-\partial^2 - M^2)\phi(x) = 0. \tag{5.765}$$

This equation can be applied to the first functional derivative of $Z[j]$:

$$\frac{\delta Z[j]}{\delta j(x)} = \langle 0|T\phi(x)e^{i\int d^4y j(y)\phi(y)}|0\rangle, \tag{5.766}$$

to find the differential equation

$$(-\partial^2 - M^2)\frac{\delta Z[j]}{\delta j(x)} = -ij(x)Z[j]. \tag{5.767}$$

That this equation must be correct is seen by integrating it functionally with the initial condition

$$Z[0] = 1, \tag{5.768}$$

and reproducing the known equation (5.764) with $G(x,y) = i/(-\partial^2 - M^2)$. A direct proof of the differential equation (5.767) proceeds by expanding both sides in a Taylor series in $j(x)$ and processing every expansion term as in (5.40)–(5.42). If we were able to pass $(-\partial^2 - m^2)$ through the time-ordering operation, we would obtain zero. During the passage, however, ∂_0^2 encounters the Heaviside function $\Theta(x_0 - x'_0)$ of the time ordering which generates additional terms. These are collected by the right-hand side of (5.767). The nth power expansion term of $Z[j]$ contributes on the left-hand side a term $nT\phi(x)[\int dz j(z)\phi(z)]^{n-1}/n!$. Applying $(-\partial^2 - m^2)$ and using the steps (5.40)–(5.42), we obtain n times a canonical commutator beween $\dot{\phi}(x)$ and $\phi(z)$ which can be written as $-j(x)T[\int dz j(z)\phi(z)]^{n-2}/(n-2)!$. Summing these up gives $-jZ[j]$. These properties will find extensive use in Chapter 12.

The formulas can be generalized to complex fields by using the generating functionals

$$\begin{aligned} O[j,j^\dagger] &= e^{i\int d^4x[j^\dagger(x)\phi(x)+j(x)\phi^\dagger(x)]}, \\ T[j,j^\dagger] &= Te^{i\int d^4x[j^\dagger(x)\phi(x)+j(x)\phi^\dagger(x)]}, \\ N[j,j^\dagger] &= Ne^{i\int d^4x[j^\dagger(x)\phi(x)+j(x)\phi^\dagger(x)]}. \end{aligned} \tag{5.769}$$

Note that for fermions, the interaction $j^\dagger(x)\phi(x)$ is odd under complex conjugation, just as for real anticommuting fields in (5.748).

Now the propagators of n fields ϕ and m fields $\phi^\dagger$ are obtained from the expectation value

$$Z[j,j^\dagger] = \langle 0|T[j,j^\dagger]|0\rangle \tag{5.770}$$

as the functional derivatives

$$\begin{aligned} &G^{(n,m)}(x_1,\dots,x_n;y_1\dots y_m) = \\ &\qquad (-i)^{m+n}\frac{\delta}{\delta j^\dagger(x_1)}\cdots\frac{\delta}{\delta j^\dagger(x_n)}\frac{\delta}{\delta j(y_1)}\cdots\frac{\delta}{j(y_m)}Z[j,j^\dagger]\bigg|_{j(x)\equiv 0}. \end{aligned} \tag{5.771}$$

The explicit form of the generating functional $Z[j,j^\dagger]$ is

$$Z[j,j^\dagger] = e^{-\int d^4x d^4y j^\dagger(x)G(x,y)j(y)}. \tag{5.772}$$

The latter form is valid for fermions if one uses anticommuting currents $j(x)$, $j^\dagger(x)$.

5.13.1 Thermodynamic Version of Wick's Theorem

In analogy with the generalization of the one-particle Green function (5.696) to the n-point functions $G^{(n)}$ of (5.698) it is useful to generalize also the thermal propagator (2.358) in an analogous way. We shall treat here explictly only the nonrelativistic case. The generalization to relativistic fields is straight-forward.

For this we introduce the thermal average for of the imaginary-time-ordered product of $n+n'$ fields:

$$G^{(n,n')}(x_1,\tau_1,\dots,x_n,\tau_n;x_1',\tau_1',\dots,x_n',\tau_n') \\ = \frac{\mathrm{Tr}\left[e^{-H_G/k_BT}T_\tau\left(\psi(x_1,\tau_1)\cdots\psi(x_n,\tau_n)\psi^\dagger(x_1',\tau_1')\cdots\psi^\dagger(x_n',\tau_n')\right)\right]}{\mathrm{Tr}\left[e^{-H_G/k_BT}\right]}, \quad (5.773)$$

where the free fields are expanded as in (2.367):

$$\psi(\mathbf{x},\tau) = \int d^3p\, f_{\mathbf{p}}(\mathbf{x},\tau)a_{\mathbf{p}}, \quad (5.774)$$

$$\psi^\dagger(\mathbf{x},\tau) = \int d^3p\, f^*_{\mathbf{p}}(\mathbf{x},\tau)a^\dagger_{\mathbf{p}}, \quad (5.775)$$

with the wave functions

$$f_{\mathbf{p}}(\mathbf{x},\tau) \equiv e^{i[\mathbf{px}-\xi(\mathbf{p})\tau]/\hbar} \equiv f^*_{\mathbf{p}}(\mathbf{x},-\tau), \qquad \xi(\mathbf{p}) = \varepsilon(\mathbf{p})-\mu, \quad (5.776)$$

where μ is the chemical potential. We shall write all subsequent equations with an explicit $\hbar$. An explicit evaluation of $G^{(n,n')}$ is much more involved than for vacuum expectation values. It proceeds using Wick's theorem, expanding $G^{(n,n')}$ into a sum of products of two-particle thermal propagators, the sum running over all possible pair contractions, just as in Eq. (5.724) for the n-point function in the vacuum. All thermal information is therefore contained in the one-particle propagators which have the Fourier decomposition (2.380) with (2.379). The detailed form will here be irrelevant.

To prove now Wick's expansion we first observe that the free Hamiltonian conserves the particle number so that $G^{(n,n')}$ vanishes unless $n=n'$. As a next step we order the product of field operators according to their imaginary time arguments τ_n thereby picking up some sign factor ±1 depending on the number of transpositions of Fermi fields. On the right-hand side of Wick's expansion the corresponding permutations lead to the same sign. Thus we may assume all field operators to be time-ordered. The ordering in τ yields a product in which the fields ψ and $\psi^\dagger$ appear in a mixed fashion. We expand each field as $\int d^3p\, f_{\mathbf{p}}\alpha_{\mathbf{p}}$, using the same notation for $\alpha_{\mathbf{p}} = a_{\mathbf{p}}$ and $\alpha_{\mathbf{p}} = a^\dagger_{\mathbf{p}}$, with the tacit understanding that in the latter case the wave function is taken as $f^*_{\mathbf{p}}$ rather than $f_{\mathbf{p}}$. Expanding the product of field operators in this way we have

$$\begin{aligned} G^{(n,n)} &= \int d^3p_1\cdots d^3p_{2n}\, f_1\cdots f_{2n} \\ &= \mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_1\cdots\alpha_{2n}\right)/\mathrm{Tr}\left(e^{-H_G/k_BT}\right), \end{aligned} \quad (5.777)$$

where we have omitted the momentum labels on the operators α, using only their numeric subscripts. There are always equally many creators as annihilators among the α_i's. In order to reduce the traces to a pure number, let us commute or anticommute α_1 successively to the right via

$$\begin{aligned} \alpha_1\alpha_2\alpha_3\ldots\alpha_{2n} &= [\alpha_1,\alpha_2]_\mp\alpha_3\cdots\alpha_{2n} \\ &\quad\pm\alpha_2[\alpha_1,\alpha_3]_\mp\alpha_4\cdots\alpha_{2n} \\ &\quad+\cdots \\ &\quad+\alpha_2\alpha_3\cdots[\alpha_1,\alpha_{2n}]_\mp \\ &\quad\pm\alpha_2\alpha_3\cdots\alpha_{2n}\alpha_1. \end{aligned} \tag{5.778}$$

The commutators or anticommutators among α_1 and α_i will give 0, if both are creators or annihilators, 1 if α_1 is an annihilator and α_i a creator, and ∓1 in the opposite case. At any rate, they are c-numbers, so that they may be taken out of the trace so that

$$\begin{aligned} &\mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_1\alpha_2\cdots\alpha_{2n}\right)\mp\mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_2\cdots\alpha_{2n}\alpha_1\right) \\ &\quad=[\alpha_1,\alpha_2]_\mp\mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_3\alpha_4\cdots\alpha_{2n}\right)\pm[\alpha_1,\alpha_3]_\mp\mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_2\alpha_4\cdots\alpha_{2n}\right) \\ &\quad+\cdots+[\alpha_1,\alpha_{2n}]_\mp\mathrm{Tr}\left(e^{H_G/k_BT}\alpha_2\alpha_3\cdots\alpha_{2n-1}\right). \end{aligned} \tag{5.779}$$

Now we make use of the cyclic property of the trace and observe that

$$\alpha_1e^{-H_G/k_BT}=e^{-H_G/k_BT}\alpha_1e^{\eta\xi(\mathbf{p})/k_BT} \tag{5.780}$$

where the sign factor $\eta=\pm1$ depends on whether α_1 is a creator or an annihilator, respectively. Then we can rewrite the left-hand side in (5.779) as

$$\left(1\mp e^{\eta\xi(\mathbf{p})/k_BT}\right)\mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_2\cdots\alpha_{2n}\alpha_1\right). \tag{5.781}$$

Dividing the prefactor out, we obtain

$$\begin{aligned} \mathrm{Tr}\left(e^{-H_G/k_BT}\alpha_1\cdots\alpha_{2n}\right) &= \mathrm{Tr}\left(e^{-H_G/k_BT}\dot\alpha_1\dot\alpha_2\alpha_3\cdots\alpha_{2n}\right) \\ &+ \mathrm{Tr}\left(e^{H_G/k_BT}\dot\alpha_1\alpha_2\dot\alpha_3\cdots\alpha_{2n}\right) \\ &+ \cdots \\ &+ \mathrm{Tr}\left(e^{-H_G/k_BT}\dot\alpha_1\alpha_2\alpha_3\cdots\dot\alpha_{2n}\right), \end{aligned} \tag{5.782}$$

where a contraction is now defined as

$$\dot\alpha_1\dot\alpha_i=\frac{[\alpha_1,\alpha_i]_\mp}{1\mp e^{\eta\xi(\mathbf{p})/k_BT}}, \tag{5.783}$$

with the same rules of taking these c-numbers outside the trace as in the ordinary Wick's theorem.

These contractions are just the Fourier transforms of the one-particle thermal propagators as given in (2.370) and (2.371). For if α_1 and α_i are both creators or annihilators, this is trivially true: both expressions vanish identically. If α_1 is an annihilator and α_i a creator, we see that [recalling (2.369) and (2.372)]

$$\dot{\alpha}_1\dot{\alpha}_i = \frac{[a_{\mathbf{p}}, a^\dagger_{\mathbf{p}'}]_\mp}{1 \mp e^{-\xi(\mathbf{p})/k_BT}} = \delta^{(3)}(\mathbf{p}-\mathbf{p}')(1 \pm n_{\xi(\mathbf{p})}). \tag{5.784}$$

In the opposite case

$$\dot{\alpha}_1\dot{\alpha}_i = \frac{[a^\dagger_{\mathbf{p}}, a_{\mathbf{p}'}]_\mp}{1 \mp e^{\xi(\mathbf{p})/k_BT}} = \delta^{(3)}(\mathbf{p}-\mathbf{p}')n_{\xi(\mathbf{p})}. \tag{5.785}$$

Multiplying either of these expressions by the product of wave functions $f_{\mathbf{p}}(\mathbf{x})f^*_{\mathbf{p}'}(\mathbf{x})$, and integrating everything over the entire momentum space, we find that these contractions are precisely the propagators $G(\mathbf{x},\tau;\mathbf{x}',\tau') = G(\mathbf{x}-\mathbf{x}',\tau-\tau')$:

$$\dot{\psi}(\mathbf{x},\tau)\dot{\psi}^\dagger(\mathbf{x}',\tau') = \pm\dot{\psi}^\dagger(\mathbf{x}',\tau')\dot{\psi}(\mathbf{x},\tau) = G(\mathbf{x}-\mathbf{x}',\tau-\tau'). \tag{5.786}$$

In (5.782), the n-particle thermal Green function $G^{(n,n)}$ has been reduced to a sum of $(n-1)$-particle propagators, each multiplied by an ordinary propagator. Continuing this procedure iteratively we arrive at Wick's expansion fot thermal Green functions.

As before, this result can be expressed most concisely in a functional form. For this we introduce

$$Z[j,j^\dagger] = \mathrm{Tr}\left(e^{-H_G/k_BT}T_\tau e^{i\int d^3x\,d\tau[j(\mathbf{x},\tau)\psi^\dagger(\mathbf{x},\tau)+\psi(\mathbf{x},\tau)j^\dagger(\mathbf{x},\tau)]}\right)/\mathrm{Tr}\left(e^{-H_G/k_BT}\right) \tag{5.787}$$

as the generating functional of thermal Green functions. Then Wick's expansion amounts to the statement

$$Z[i,j^\dagger] = e^{-\int d^3x\,d\tau d^3x'd\tau' j^\dagger(\mathbf{x},\tau)G(\mathbf{x}-\mathbf{x}',\tau-\tau')j(\mathbf{x},\tau)} \tag{5.788}$$

As before, this can be derived from the equation of motion [compare (2.365) and (2.366)]

$$\begin{aligned}\left(-\partial_\tau + \frac{\boldsymbol{\nabla}^2}{2M} + \mu\right)\frac{\delta}{\delta j^\dagger(\mathbf{x},\tau)}Z[j,j^\dagger] &= -Z[j,j^\dagger]j(\mathbf{x},\tau),\\ Z[j,j^\dagger]\frac{\overleftarrow{\delta}}{\delta j(\mathbf{x},\tau)}\left(-\overleftarrow{\partial}_\tau + \frac{\overleftarrow{\boldsymbol{\nabla}}^2}{2M} + \mu\right) &= -j^\dagger(\mathbf{x},\tau)Z[j,j^\dagger],\end{aligned} \tag{5.789}$$

following the procedure to prove Eq. (5.767). Here the proof is simpler since only one time derivative needs to be passed through the time-ordering operation T_τ producing a canonical equal-time commutator for every pair of fields, as in (2.239). As a check we integrate again (5.789) with the initial condition $Z[0,0] = 1$, and recover (5.788).

It is worth deriving also a related theorem concerning the thermal expectations of normally ordered field operators. According to Wick's theorem in the operator form (5.723), any product of time ordered operators can be expanded into normal products, so that

$$Z[j,j^\dagger] = e^{-\int d^4x d^4x' j^\dagger(x)G(x-x')j(x)} \times \frac{\mathrm{Tr}\left(e^{-H_G/k_BT} N e^{i\int d^4x[j^\dagger(x)\psi(x)+\psi^\dagger(x)j(x)]}\right)}{\mathrm{Tr}\,(e^{-H_G/k_BT})}, \tag{5.790}$$

where we have used the four-vector notation $x = (\mathbf{x}, \tau)$ and $d^4x = d^3x\,d\tau$, for brevity. We can show that the expectation of the normal product can be expanded once more in a Wick-like way. For this we introduce expectation of two normally ordered operators

$$G_N(x_1,x_2) \equiv \frac{\mathrm{Tr}\left[e^{-H_G/k_BT} N\left(\psi^\dagger(x_1)\psi(x_2)\right]\right)}{\mathrm{Tr}\left[e^{-H_G/k_BT}\right]}. \tag{5.791}$$

This quantity can be calculated by inserting (5.774) and (5.775), as well as intermediate states, with the result

$$G_N(x_1,x_2) = \int \bar{d}^3p\, e^{i[\mathbf{p}(\mathbf{x}_2-\mathbf{x}_1)+i\xi(\mathbf{p})(\tau_1-\tau_2)]/\hbar} n_{\xi(\mathbf{p})}, \tag{5.792}$$

where n_ξ is the particle distribution function for bosons and fermions, respectively:

$$n_\xi = \frac{1}{e^{\xi/k_BT} \pm 1}. \tag{5.793}$$

It can now be shown that the thrmal expectation value of an arbitrary normal product can be expanded into expectation values of the one-particle normal products (5.791) in the same way as the τ-ordered product into the expectations of one-particle τ-ordered propagators. The proof is most easily given functionally. We consider the generating functional

$$N[j,j^\dagger] \equiv \mathrm{Tr}\left(e^{-H_G/k_BT} N e^{i\int d^4x(\psi^\dagger(x)j(x)+j^\dagger(x)\psi(x))}\right)/\mathrm{Tr}\left(e^{-H_G/k_BT}\right) \tag{5.794}$$

and differentiate this with respect to $j^\dagger(x)$:

$$\frac{\delta N[j,j^\dagger]}{i\delta j^\dagger(x)} = \mathrm{Tr}\left[e^{-H_G/k_BT} N\left(\psi(x)e^{i\int d^4x(\psi^\dagger j+j^\dagger\psi)}\right)\right]/\mathrm{Tr}\left[e^{-H_G/k_BT}\right]. \tag{5.795}$$

Applying to this the field equation

$$\left(-\partial_\tau + \frac{\boldsymbol{\nabla}^2}{2M} + \mu\right)\psi(x) = 0, \tag{5.796}$$

we see that $N[j,j^\dagger]$ satisfies

$$\left(-\partial_\tau + \frac{\boldsymbol{\nabla}^2}{2M} + \mu\right)\frac{\delta}{\delta j^\dagger} N[j,j^\dagger] = 0. \tag{5.797}$$

This is solved by

$$N[j,j^\dagger] = e^{-\int d^4x_1 d^4x_2 j^\dagger(x_1) G_N(x_1,x_2) j(x_2)} \tag{5.798}$$

where $G_N(x_1,x_2)$ is a solution of the homogeneous differential equation. To obtain the correct result for the ordinary imaginary-time propagator, we expand both sides in $j, j^\dagger$ and see that $G_N(x_1,x_2)$ coincides with (5.791), (5.792).

Appendix 5A Liénard-Wiechert Potential

Let us calculate the field around a point source with a time-dependent position $\bar{\mathbf{x}}(t)$, whose current is

$$j(t',\mathbf{x}') = \int d\tau \delta^{(4)}(x' - \bar{x}(\tau)) = \frac{1}{d\bar{x}_0/d\tau} \delta^{(3)}(\mathbf{x}' - \bar{\mathbf{x}}(t')), \tag{5A.1}$$

where τ is the proper time, and $d\bar{x}^0/d\tau = \sqrt{1-\bar{\mathbf{v}}^2(t)} = \gamma(t)$, with $\bar{\mathbf{v}}(t)$ being is the velocity along the trajectory $\bar{\mathbf{x}}(t)$:

$$\bar{\mathbf{v}}(t) \equiv \dot{\bar{\mathbf{x}}}(t). \tag{5A.2}$$

After performing the spatial integral in (5.181) we obtain

$$\phi(\mathbf{x},t) = \int dt' \, \Theta(t-t') \frac{1}{4\pi R} \frac{1}{\gamma} \delta(t-t'-R(t')), \tag{5A.3}$$

where $R(t)$ is the distance from the moving source position at the time t:

$$R(t') = |\mathbf{x} - \bar{\mathbf{x}}(t')|. \tag{5A.4}$$

The integral over t' gives a contribution only for $t' = t_R$ determined from t by the retardation condition

$$t - t_R - R(t_R) = 0. \tag{5A.5}$$

At that point, the δ-function can be rewritten as

$$\delta(t-t'-R(t')) = \frac{1}{|d[t'+R(t')]/dt'|_{t'=t_R}} \delta(t'-t_R) = \frac{1}{1-\mathbf{n}(t_R)\cdot\bar{\mathbf{v}}(t_R)} \delta(t'-t_R), \tag{5A.6}$$

where $\mathbf{n}(t)$ is the direction of the distance vector from the charge.

$$\mathbf{n}(t) \equiv \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|} \tag{5A.7}$$

Thus we find the Liénard-Wiechert-like potential:

$$\phi(\mathbf{x},t) = -\left[\frac{1}{\gamma(1-\mathbf{n}\cdot\bar{\mathbf{v}})R}\right]_{\text{ret}}. \tag{5A.8}$$

and the *retarded distance* from the point source

$$R_{\text{ret}}(t) = |\mathbf{x} - \bar{\mathbf{x}}(t_R)|. \tag{5A.9}$$

Appendix 5B Equal-Time Commutator from Time-Ordered Product

As an exercise in handling the functions in Section 5.2, consider the relationship between the commutator at equal-times and the time-ordered product. The first can be obtained from the latter by forming the difference

$$[\phi(x),\phi(x')]_{x^0-x'^0}=T(\phi(x)\phi(x'))|_{x^0-x'^0=\epsilon}-T(\phi(x)\phi(x'))|_{x^0-x'^0=-\epsilon},\tag{5B.1}$$

where ϵ is an infinitesimal positive time. Thus, the Fourier representation of the equal-time commutator is obtained from that of the Feynman propagator by replacing in the p^0-integral of (5.63) the exponential $e^{-ip^0(x^0-x'^0)}$ by $e^{-ip^0\epsilon}-e^{ip^0\epsilon}$. Thus we should get for the commutator function at equal times

$$C(x-x')|_{x^0=x'^0}=\int\frac{d^3p}{(2\pi)^3}e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')}\int\frac{dp^0}{2\pi}(e^{-ip^0\epsilon}-e^{ip^0\epsilon})\frac{i}{p^2-M^2+i\eta}.\tag{5B.2}$$

The p^0-integral can now be performed by closing the contour in the first term by a semicircle in the lower halfplane, in the second term by one in the upper halfplane. To do this, we express the Feynman propagator via the first of the rules (5.202) [see also (5.189)] as

$$\frac{i}{p^2-M^2+i\eta}=\pi\delta_-(p^2-M^2)=\pi\delta_-(p^{02}-\omega_{\mathbf{p}}^2),\tag{5B.3}$$

and use the simple integrals

$$\int_{-\infty}^{\infty}\frac{dp^0}{2\pi}e^{-ip^0\epsilon}\pi\delta_-(p^0-\omega_{\mathbf{p}})=1,\qquad\int_{-\infty}^{\infty}\frac{dp^0}{2\pi}e^{-ip^0\epsilon}\pi\delta_+(p^0+\omega_{\mathbf{p}})=0,\tag{5B.4}$$

$$\int_{-\infty}^{\infty}\frac{dp^0}{2\pi}\,e^{ip^0\epsilon}\,\pi\delta_-(p^0-\omega_{\mathbf{p}})=0,\qquad\int_{-\infty}^{\infty}\frac{dp^0}{2\pi}\,e^{ip^0\epsilon}\pi\delta_+(p^0+\omega_{\mathbf{p}})=1.\tag{5B.5}$$

to find a vanishing commutator function.

For its time derivative, These imply that exponentials $e^{\mp ip^0\epsilon}$ together with $\delta_-(p^0-\omega_{\mathbf{p}})$ and $\delta_+(p^0-\omega_{\mathbf{p}})$ have the same effect as Heaviside functions $\Theta(\pm p^0)$ accompanied by $2\pi\delta_\pm(p^0-\omega_{\mathbf{p}})$ and $2\pi\delta_\pm(p^0+\omega_{\mathbf{p}})$, respectively. We can therefore replace in the p^0-integral of the Fourier representation (5B.2) of the commutator function

$$\int\frac{dp^0}{2\pi}(e^{-ip^0\epsilon}-e^{ip^0\epsilon})\frac{i}{p^2-M^2+i\eta}\to\int\frac{dp^0}{2\pi}\left[\Theta(p^0)-\Theta(-p^0)\right]2\pi\delta(p^2-M^2),\tag{5B.6}$$

and this is the same as the p^0-integral in Eq. (5.196) for $C(x-x')$ at equal times, which vanishes.

For the time derivative of the commutator function $C(x-x')$, the integrand carries an extra factor $-p^0$, and (5B.7) becomes

$$\int\frac{dp^0}{2\pi}(-ip^0)(e^{-ip^0\epsilon}-e^{ip^0\epsilon})\frac{i}{p^2-M^2+i\eta}\to-i\int\frac{dp^0}{2\pi}\omega_{\mathbf{p}}2\pi\delta(p^2-M^2)=-i,\tag{5B.7}$$

so that we find the correct result $\dot{C}(-x')_{x^0-x'^0} = -i\delta^{(3)}(x-x')$.

With the same formalism one may also check the consistency of the photon propagator (5.524) with the commutation rules (5.527)–(5.530). As in (5B.1), we write

$$\begin{aligned}[A^\mu(x), A^\nu(x')]|_{x^0=x'^0} &= \int \frac{d^4k}{(2\pi)^4}(e^{-ik^0\epsilon} - e^{ik^0\epsilon})e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\frac{i}{k^2+i\eta} \\ &\times \left[-g^{\mu\nu} + (1-\alpha)\frac{k^\mu k^\nu}{k^2+i\eta}\right] \qquad (5B.8)\end{aligned}$$

The contribution of $-g^{\mu\nu}$ in the brackets yields the commutator function $C(x-x')$ of the scalar field. The second contribution proportional to $k^\mu k^\nu$ is nontrivial. First we insert

$$\frac{1}{k^2+i\eta} = \delta_+(k^2) = \frac{1}{2\omega_{\mathbf{k}}}[\delta_+(k^0-\omega_{\mathbf{k}}) + \delta_+(k^0+\omega_{\mathbf{k}})],$$

with $\omega_{\mathbf{k}} = |\mathbf{k}|$. By forming the derivative ∂_μ and taking $\nu = 0$, the first term gives

$$i\delta^{(3)}(\mathbf{x}-\mathbf{x}').$$

The second term is equal to

$$-i(1-\alpha)\int \frac{d^4k}{(2\pi)^4}(e^{-ik^0\epsilon} - e^{ik^0\epsilon})e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\frac{1}{2\omega_{\mathbf{k}}}[\delta_+(k^0-\omega_{\mathbf{k}}) + \delta_+(k^0+\omega_{\mathbf{k}})]k^0 \qquad (5B.9)$$

Since k^0 changes the relative sign of the two pole contributions, the k-integration gives

$$-i(1-\alpha)\delta^{(3)}(\mathbf{x}-\mathbf{x}')$$

leading to the equal-time commutator

$$[\partial_\mu A^\mu(x), A^0(x')]|_{x_0=x'^0} = i\alpha\delta^{(3)}(\mathbf{x}-\mathbf{x}') \qquad (5B.10)$$

in agreement with (5.527), provided that

$$[\partial_i A^i(x), A^0(x')]|_{x_0=x'^0} = 0. \qquad (5B.11)$$

This commutator has the a spectral decomposition coming only from the second term in (5B.8): It is equal to

$$\begin{aligned}&-i(1-\alpha)\int \frac{d^4k}{(2\pi)^4}(e^{-ik^0\epsilon} - e^{ik^0\epsilon})e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\frac{1}{2k^0}[\delta_+(k^0-\omega_{\mathbf{k}}) + \delta_+(k^0+\omega_{\mathbf{k}})] \\ &\qquad \times\mathbf{k}^2 k^0\frac{1}{2\omega_{\mathbf{k}}}[\delta_+(k^0-\omega_{\mathbf{k}}) + \delta_+(k^0+\omega_{\mathbf{k}})] \qquad (5B.12)\end{aligned}$$

By writing

$$k^0\frac{1}{2\omega_{\mathbf{k}}}[\delta_+(k^0-\omega_{\mathbf{k}}) + \delta_+(k^0+\omega_{\mathbf{k}})] = k^0\frac{1}{2\omega_{\mathbf{k}}}[\delta_+(k^0-\omega_{\mathbf{k}}) - \delta_+(k^0+\omega_{\mathbf{k}})]$$

we see that the δ_+-functions appear in the combination $[\delta_+(k^0-\omega_{\mathbf{k}})]^2-[\delta_+(k^0+\omega_{\mathbf{k}})]^2$. When closing the integration contours in the upper or lower k^0-plane, the double-poles give no contribution. Hence

$$[\partial_i A^i(x), A^0(x')]|_{x0=x'0} = 0. \tag{5B.13}$$

For the same reason, the commutators $[\dot{A}^i(x), \dot{A}^j(x')]|_{x0=x'0}$ receive only a contribution from the first term and yield $-i\delta_{ij}\delta^{(3)}(\mathbf{x}-\mathbf{x}')$. Other commutators are

$$\begin{aligned}[D(x), \dot{A}^i(x')]|_{x0=x'0} &= -[D(x), \partial_i A^0(x')]|_{x0=x'0}\\ &= \int \frac{d^4k}{(2\pi)^4}(e^{-ik^0\epsilon}-e^{ik^0\epsilon})e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\frac{i}{k^2+i\eta}\alpha k^i k^0 \end{aligned} \tag{5B.14}$$

yielding

$$\alpha i\delta^{(3)}(\mathbf{x}-\mathbf{x}')$$

which shows that $D(x)$ commutes with $E^i(x)$ at equal times. Together with the previous result we recover the third of the canonical commutators (5.527)–(5.530).

Appendix 5C Euler-Maclaurin formula

The Euler-Maclaurin formula which serves to calculate discrete sums such as that in Eq. 5.669) can be derived from a fundamental summation formula due to Bernoulli. Just as a power n^p is integrated to

$$\int_N^M dn\, n^p = \frac{b_{p+1}(M)-b_{p+1}(N)}{p+1}, \tag{5C.1}$$

where $b_{p+1}(x)\equiv x^{p+1}$, the corresponding sum over integers is given by sums over integer numbers are given by *Bernoulli polynomials* $B_p(x)$ as follows:

$$\sum_{n=N}^{M} n^p = \frac{B_{p+1}(M+1)-B_{p+1}(N)}{p+1}, \tag{5C.2}$$

where $B_p(x)$ are *Bernoulli polynomials*:

$$\begin{aligned} B_0(x) &\equiv 1,\\ B_1(x) &= -\frac{1}{2}+x,\\ B_2(x) &= \frac{1}{6}-x+x^2,\\ B_3(x) &= \frac{1}{2}x-\frac{3}{2}x^2+x^3,\\ B_4(x) &= -\frac{1}{30}+x^2-2x^3+x^4,\\ B_5(x) &= -\frac{1}{6}x+\frac{5}{3}x^3-\frac{5}{2}x^4+x^5,\\ &\vdots \end{aligned} \tag{5C.3}$$

The more general integral

$$\int_N^M dn\,(n+x)^p = \frac{b_{p+1}(M+x)-b_{p+1}(N+x)}{p+1} \tag{5C.4}$$

reads for a sum:

$$\sum_{n=N}^{M}(n+x)^p = \frac{B_{p+1}(M+1+x)-B_{p+1}(N+x)}{p+1}. \tag{5C.5}$$

The values of the polynomials $B_p(x)$ at $x=0$ are called *Bernoulli numbers* B_p:

$$B_0=1,\ B_1=-\frac{1}{2},\ B_2=\frac{1}{6},\ B_3=0,\ B_4=-\frac{1}{30},\ B_5=0,\ B_6=\frac{1}{42},\ \dots\ . \tag{5C.6}$$

Except for B_1, all odd Bernoulli numbers vanish.

The close correspondence between integrals and sums has its counterpart in differential and difference equations: By differentiating $b_p(x)=x^p$, we find:

$$b'_p(x)=px^{p-1}, \tag{5C.7}$$

whereas Eqs. (5C.2) and (5C.5) follow from an analogous difference equation

$$B_p(x+1)-B_p(x)=px^{p-1}, \tag{5C.8}$$

and the initial condition

$$B_0(x)\equiv 1. \tag{5C.9}$$

The differential relation

$$b'_p(x)=pb_{p-1}(x) \tag{5C.10}$$

is completely shared by $B_p(x)$:

$$B'_p(x)=pB_{p-1}(x). \tag{5C.11}$$

There is another important property of the function $b_p(x)=x^p$, the binomial expansion of $(x+h)^p$

$$b_p(x+h)=\sum_{q=0}^{p}\binom{p}{q}b_q(x)h^{p-q}, \tag{5C.12}$$

which is shared by $B_p(x)$:

$$B_p(x+h)=\sum_{n=0}^{p}\binom{p}{n}B_n(x)h^{p-n}, \tag{5C.13}$$

A noncommon property of the Bernoulli polynomials which is caused by the discrete nature of the sum is

$$B_p(1-x)=(-1)^pB_p(x). \tag{5C.14}$$

There exists a simple generating function for the Bernoulli polynomials which ensures the fundamental property (5C.8):

$$\frac{te^{xt}}{e^t-1}=\sum_{p=0}^{\infty}B_p(x)\frac{t^p}{p!}. \tag{5C.15}$$

The property (5C.5) can directly be used to calculate the difference between an integral and a discrete sum over a function $F(t)$. If an interval $t \in (a,b)$ is divided into m slices of width $h=(b-a)/N$, we obviously have

$$h\sum_{n=0}^{N-1}F(a+(n+x)h)-\int_a^b dt\,F(t)=\sum_{p=1}^{\infty}\frac{h^p}{p!}[B_p(N+x)-B_p(x)]F^{(p-1)}(a). \tag{5C.16}$$

This follows from expanding the left-hand side into powers of h. After this, the binomial expansion (5C.29) leads to

$$\begin{aligned}\sum_{p=1}^{\infty}\frac{h^p}{p!}B_p(x+N+1)F^{(p-1)}(a) &= \sum_{p=1}^{\infty}\sum_{l=0}^{p}\frac{h^p}{p!}\binom{p}{l}B_l(x)\,N^{p-l}F^{(p-1)}(a)\\ &= \sum_{l=0}^{p}\frac{h^l}{l!}B_l(x)\sum_{p=l}^{\infty}\frac{1}{(p-l)!}(hN)^{p-l}F^{(p-1)}(a)\\ &= \sum_{l=0}^{p}\frac{h^l}{l!}B_l(x)F^{(l-1)}(b),\end{aligned} \tag{5C.17}$$

which brings (5C.16) to *Euler's formula*

$$h\sum_{n=0}^{N-1}F(a+(n+x)h)-\int_a^b dt\,F(t)=\sum_{p=1}^{\infty}\frac{h^p}{p!}B_p(x)[F^{(p-1)}(b)-F^{(p-1)}(a)]. \tag{5C.18}$$

Since all off Bernoulli numbers vanish except for $B_1=-1/2$, it is useful to remove the $p=1$ -term from the right-hand side and rewrite (5C.25) as

$$\begin{aligned}h\sum_{n=0}^{N-1}F(a+(n+x)h)-\int_a^b dt\,F(t) &= (-1/2+x)\,[F(b)-F(a)]\\ &+\sum_{p=1}^{\infty}\frac{h^{2p}}{(2p)!}B_{2p}(x)[F^{(2p-1)}(b)-F^{(2p-1)}(a)].\end{aligned} \tag{5C.19}$$

For $x=0$ we may extend the sum on the left-hand side to $n=N$ and obtain the *Euler-Maclaurin* formula:[37]

$$\begin{aligned}h\sum_{n=0}^{N}F(a+nh)-\int_a^b dt\,F(t) &= \frac{1}{2}\,[F(b)+F(a)]\\ &+\sum_{p=1}^{\infty}\frac{h^{2p}}{(2p)!}B_{2p}(x)[F^{(2p-1)}(b)-F^{(2p-1)}(a)].\end{aligned} \tag{5C.20}$$

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[37] See M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Eqs. 23.1.30 and 23.1.32.

If the sums (5C.5) are carried to infinity, they diverge. These infinities may, however, be removed by considering such sums as a analytic continuations of convergent sums

$$\zeta(z,x) \equiv \sum_{n=0}^{\infty} \frac{1}{(n+x)^z}, \qquad \mathrm{Re}\, z > 1. \tag{5C.21}$$

known as *Riemann's zeta functions*. A continuation is possible by an appropriate deformation of the contour in the integral representation

$$\zeta(z,x) = \frac{1}{\Gamma(z)} \int_0^\infty \frac{t^{z-1}e^{-xt}}{1-e^{-t}}. \tag{5C.22}$$

This yields the relation:

$$\zeta(-p,x) = -\frac{B_{p+1}(x)}{p+1} \tag{5C.23}$$

Thus the finite sum (5C.5) can be understood as the difference between the regularized infinite sums

$$\begin{aligned} \sum_{n=0}^{\infty}(n+x)^p &= \zeta(-p,x) = -\frac{B_{p+1}(x)}{p+1}, \\ \text{and} \qquad \sum_{n=m+1}^{\infty}(n+x)^p &= \zeta(-p,m+x) = -\frac{B_{p+1}(m+1+x)}{p+1}. \end{aligned} \tag{5C.24}$$

With the help of these regularized infinite sums we can derive Euler's formula (5C.25) by considering the left-hand side as a difference between the infinite sum

$$\left[h\sum_{n=0}^{\infty} F(a+(n+x)h) - \int_a^\infty dt\, F(t)\right] \tag{5C.25}$$

and a corresponding sum for b instead of a. By expanding each sum in a powers of h and using the formula (5C.24), we find directly (5C.25).

For completeness, let us mention that alternating sums are governed quite similarly by *Euler polynomials*

$$\sum_{n=N}^{M}(-1)^{m-n}(n+x)^n = \frac{E_{n+1}(M+1+x)+(-1)^m E_{n+1}(p+x)}{2}, \tag{5C.26}$$

and $E_n \equiv 2^n E_n(1/2)$ are called *Euler numbers*:[38]

$$E_0 = 1,\ E_1 = 0,\ E_2 = -1,\ E_3 = 0,\ E_4 = 5,\ E_5 = 0,\ E_6 = -61\ \dots\ . \tag{5C.27}$$

All odd Euler numbers vanish. The Euler polynomials satisfy

$$E_p(x+1)+E_p(x) = 2x^{p-2},\ \ E_p'(x) = pE_{p-1}(x),\ \ E_p(1-x) = (-1)^p E_p(x) \tag{5C.28}$$

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[38] Note the difference with respect to the definition of the Bernoulli numbers (5C.6) which are defined by the values of $B_n(x)$ at $x = 0$.

and

$$E_p(x+h) = \sum_{n=0}^{p} \binom{p}{n} E_n(x) h^{p-n}, \tag{5C.29}$$

The values $E_p(0)$ are related to the Bernoulli numbers by

$$E_p(0) = -2(2^{p+1}-1)B_{p+1}/(p+1). \tag{5C.30}$$

The generating function of the Euler polynomials is[39]

$$\frac{2e^{xt}}{e^t+1} = \sum_{n=0}^{\infty} E_p(x)\frac{t^p}{p!}. \tag{5C.31}$$

Notes and References

The Clebsch-Gordan-like reduction of two-particle states into irreducible representations of the Poincaré group is discussed in detail in
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[39] Further properties of these polynomials can be found in M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965, Chapter 23.

6

Continuous Symmetries and Conservation Laws; Noether's Theorem

In many physical systems, the action is invariant under some continuous set of transformations. Then there exist local and global conservation laws, the most important among them being the conservation of charges and currents in electrodynamics. This conservation law was observed before in Eqs. (3.165) and (3.457), but the deeper reason for its existence will only be understood in this chapter.

After quantizing the dynamical variables, the globally conserved quantities, the analogs of the charges, can be used to generate the symmetry transformation, from which they were derived, in the Hilbert space of the system.

6.1 Point Mechanics

Consider first a simple mechanical system with a generic action

$$\mathcal{A} = \int_{t_a}^{t_b} dt L(q(t), \dot{q}(t), t). \tag{6.1}$$

6.1.1 Continuous Symmetries and Conservation Law

Suppose $\mathcal{A}$ is invariant under a continuous set of variable transformations of the dynamical variables:

$$q(t) \to q'(t). \tag{6.2}$$

Then these transformations are called *symmetry transformations*. If the action is subjected successively to two symmetry transformation, the result is again a symmetry transformation. Thus the symmetry transformation form a group, the *symmetry group* of the system. It is important that the equations of motion are not used when checking this invariance.

For infinitesimal symmetry transformations (6.2), the difference

$$\delta_s q(t) \equiv q'(t) - q(t)$$

will be called a *symmetry variation*. It has the general form

$$\delta_s q(t) = \epsilon \Delta(q(t), \dot{q}(t), t) \tag{6.3}$$

Symmetry variations differ from ordinary variations $\delta q(t)$ used for deriving the Euler-Lagrange equations of motion from the principle of extremal action by not vanishing at the boundary. In contrast to $\delta q(t)$ which satisfies $\delta q(t_b) = \delta q(t_a) = 0$, the symmetry variation $\delta_s q(t)$ is nonzero at t_b and t_a.

To find the conservation law associated with this symmetry transformation, we evaluate explicitly the symmetry variation of the action implied by (6.3). Using the chain rule of differentiation and a partial integration we find

$$\delta_s \mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{\partial L}{\partial q(t)} - \partial_t \frac{\partial L}{\partial \dot{q}(t)} \right] \delta_s q(t) + \left. \frac{\partial L}{\partial \dot{q}(t)} \delta_s q(t) \right|_{t_a}^{t_b}. \tag{6.4}$$

For orbits $q(t)$ which satisfy the equations of motion, the integral vanishes and we are left with

$$\delta_s \mathcal{A} = \epsilon \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) \bigg|_{t_b}^{t_a} . \tag{6.5}$$

Since $\delta_s \mathcal{A}$ vanishes for *any* orbit $q(t)$ by assumption, this implies that the quantity

$$Q = \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) \tag{6.6}$$

This is the same at the times t_a and t_b. Since this is true for all t_b, the quantity Q is *independent* of the time t_b, i.e., it satisfies

$$\frac{d}{dt} Q(t) = 0. \tag{6.7}$$

It is a *constant of motion*, a *conserved quantity*.

The statement can be generalized to transformations $\delta_s q(t)$ for which the action is not directly invariant but equal to an arbitrary boundary term

$$\delta_s \mathcal{A} = \epsilon \Lambda(q, \dot{q}, t)|_{t_a}^{t_b}. \tag{6.8}$$

Now,

$$Q(t) = \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t) - \Lambda(q, \dot{q}, t) \tag{6.9}$$

satisfies (6.7), i.e., it is a conserved quantity.

The invariance of the action with possible surface terms is guaranteed if the Lagrangian changes under a transformation $\delta_s q(t)$ merely by a *total time derivative*:

$$\delta_s L(q, \dot{q}, t) = \epsilon \frac{d}{dt} \Lambda(q, \dot{q}, t) \tag{6.10}$$

From this property we can also derive the constant of motion also without invoking the action, directly from the Lagrangian, by expanding its symmetry variation as follows:

$$\delta_{\rm s} L \equiv L\left(q+\delta_{\rm s} q, \dot{q}+\delta_{\rm s} \dot{q}\right)-L(q, \dot{q})=\left[\frac{\partial L}{\partial q(t)}-\partial_t \frac{\partial L}{\partial \dot{q}(t)}\right] \delta_{\rm s} q(t)+\frac{d}{d t}\left[\frac{\partial L}{\partial \dot{q}(t)} \delta_{\rm s} q(t)\right] \tag{6.11}$$

As usual when dealing with infinitesimal variations, we omit all terms of higher than linear order in $\delta_{\rm s} q(t)$. On account of the equations of motion, only the last term survives. After equating (6.11) with (6.10), we find

$$\epsilon \frac{d}{d t}\left[\frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t)-\Lambda(q, \dot{q}, t)\right]=0, \tag{6.12}$$

thus recovering again the conservation law (6.7).

The existence of a conserved quantity for every continuous symmetry is the content of *Noether's theorem.*[1]

6.1.2 Alternative Derivation

From the action principle it follows that if we subject a classical orbit $q_c(t)$ which extremizes the action to an *arbitrary variation* $\delta_{\rm a} q(t)$ which does *not* vanish at the boundaries, i.e., which does not satisfy $\delta q(t_b)=\delta q(t_a)=0$, the action changes by a pure boundary term. Indeed, then the first term in the expansion

$$\delta_{\rm a} \mathcal{A}=\int_{t_a}^{t_b} d t\left[\frac{\partial L}{\partial q(t)}-\partial_t \frac{\partial L}{\partial \dot{q}(t)}\right] \delta_{\rm a} q+\left.\frac{\partial L}{\partial \dot{q}} \delta_{\rm a} q\right|_{t_a} ^{t_b} \tag{6.13}$$

vanishes and

$$\delta \mathcal{A}=\left.\frac{\partial L}{\partial \dot{q}} \delta q\right|_{t_a} ^{t_b} \tag{6.14}$$

This observation leads to another derivation of Noether's theorem. Suppose we subject a classical orbit to a variation which generalizes the symmetry transformation by containing a parameter ϵ depending on time:

$$\delta_{\rm s}^t q(t)=\epsilon(t) \Delta(q(t), \dot{q}(t), t). \tag{6.15}$$

These are called *local symmetry transformation.* The superscript t indicates the artificial time dependence in the parameter $\epsilon(t)$. These transformations may be considered as a special set of the general variations $\delta_{\rm a} q(t)$ introduced above. Thus $\delta_{\rm s}^t \mathcal{A}$ must also be a pure boundary term.

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[1] Elly Noether, Nachr. d. vgl. Ges. d. Wiss. Göttingen, Math-Phys. Klasse, 235 (1918); See also Bessel-Hagen, Math. Ann. **84**, 258 (1926); L. Rosenfeld, Me. Acad. Roy. Belg. **18**, 2 (1938); F. Belinfante, Physica **6**, 887 (1939).

For the subsequent discussion it will be useful to introduce the Lagrangian of an orbit

$$q^\epsilon(t) \equiv q(t) + \delta_{\rm s}^t q(t) \tag{6.16}$$

which differs from the classical orbit by the local symmetry variation, i.e.,

$$L^\epsilon \equiv L(q^\epsilon(t), \dot{q}^\epsilon(t)). \tag{6.17}$$

Then $\delta_{\rm s}^t \mathcal{A}$ may be calculated as follows:

$$\delta_{\rm s}^t \mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{\partial L^\epsilon}{\partial \epsilon(t)} - \frac{d}{dt} \frac{\partial L^\epsilon}{\partial \dot{\epsilon}(t)} \right] \epsilon(t) + \frac{d}{dt} \left[\frac{\partial L^\epsilon}{\partial \dot{\epsilon}} \right] \epsilon(t) \Big|_{t_a}^{t_b} \tag{6.18}$$

Since this may depend only on the boundaries, and $\epsilon(t)$ is an arbitrary small function of time, we conclude that there exists an Euler-Lagrange type of equation

$$\frac{\partial L^\epsilon}{\partial \epsilon(t)} - \frac{d}{dt} \frac{\partial L^\epsilon}{\partial \dot{\epsilon}(t)} = 0 \tag{6.19}$$

By assumption, the action was a pure surface term under t-independent transformations (6.15). This implies that

$$\frac{\partial L^\epsilon}{\partial \epsilon} = \frac{d}{dt} \Lambda. \tag{6.20}$$

In combination with (6.19), this implies the existence of a conserved charge:

$$Q = \frac{\partial L^\epsilon}{\partial \dot{\epsilon}} - \Lambda. \tag{6.21}$$

This is the same charge as (6.9). To prove this we calculate the derivative with respect to $\dot{\epsilon}$ using the chain rule

$$\begin{aligned} \frac{\partial L^\epsilon}{\partial \dot{\epsilon}} &= \frac{\partial L}{\partial q} \frac{\partial \delta q_{\rm s}^t}{\partial \dot{\epsilon}} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \delta_{\rm s}^t \dot{q}}{\partial \dot{\epsilon}} \\ &= \frac{\partial L}{\partial \dot{q}} \Delta(q, \dot{q}, t). \end{aligned} \tag{6.22}$$

Inserted into (6.21), this yields the charge (6.9).

Note that (6.22) can also be written as

$$\frac{\partial L^\epsilon}{\partial \dot{\epsilon}} = \frac{\partial L}{\partial \dot{q}} \frac{\partial \delta_{\rm s}^t q}{\partial \epsilon}. \tag{6.23}$$

6.2 Displacement and Energy Conservation

As a simple but important example consider the case that $L(q,\dot{q})$ does not depend explicitly on time. Let us perform a time translation on the coordinate frame

$$t' = t - \epsilon. \tag{6.24}$$

The negative sign is used to have a positive sign in on the right-hand side of (6.26). In the new coordinate frame, the *same* orbit has the new description

$$q'(t') = q(t), \tag{6.25}$$

i.e., the orbit $q'(t)$ at the translated time t' is precisely the same as the orbit $q(t)$ at the original time t. If we replace the argument of $q'(t)$ in (6.25) by t, we describe a time-translated orbit with the original coordinates. This implies the symmetry variation as

$$\begin{aligned}\delta_{\rm s} q(t) &= q'(t) - q(t) = q'(t'+\epsilon) - q(t)\\ &= q'(t') + \epsilon\dot{q}'(t') - q(t) = \epsilon\dot{q}(t),\end{aligned} \tag{6.26}$$

The symmetry variation of the Lagrangian is

$$\delta_{\rm s} L = L(q'(t),\dot{q}'(t)) - L(q(t),\dot{q}(t)) = \frac{\partial L}{\partial q}\delta_{\rm s} q(t) + \frac{\partial L}{\partial \dot{q}}\delta_{\rm s}\dot{q}(t). \tag{6.27}$$

Inserting the explicit $\delta_{\rm s} q(t)$ from (6.26), we find without using the Euler-Lagrange equation

$$\delta_{\rm s} L = \epsilon\left(\frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q}\right) = \epsilon\frac{d}{dt}L, \tag{6.28}$$

which is Eq. (6.10) with $\Lambda = L$. Hence, time translations are symmetry transformation.

According to Eq. (6.9), the quantity

$$Q = \frac{\partial L}{\partial \dot{q}}\dot{q} - L(q,\dot{q}) \tag{6.29}$$

is a constant of motion. This is the Legendre transform of the Lagrangian, the *Hamiltonian* of the system.

This is the same charge as that obtained from (6.9), since with

$$\delta_{\rm s}^t q(t) = \epsilon(t)\dot{q}(t) \tag{6.30}$$

implies

$$\delta_{\rm s}^t L = \frac{\partial L}{\partial q}\epsilon\dot{q} + \frac{\partial L}{\partial \dot{q}}\left(\dot{\epsilon}\dot{q} + \epsilon\ddot{q}\right), \tag{6.31}$$

so that

$$\frac{\partial L^\epsilon}{\partial \dot\epsilon} = \frac{\partial L}{\partial \dot q}\dot q \tag{6.32}$$

and

$$\frac{\partial L^\epsilon}{\partial \epsilon} = \frac{d}{dt}L. \tag{6.33}$$

Thus, Eq. (6.21) yields again the charge (6.9).

6.3 Momentum and Angular Momentum

Just as the conservation law of energy follow from the symmetry of the action under time translations, the conservation of momentum and angular momentum are a consequence of an invariance of the action under translations and rotations.

Consider a Lagrangian of a point particle in a euclidean space

$$L = L(x^i, \dot x^i) \tag{6.34}$$

in which x^i are cartesian coordinates. If the Lagrangian does not depend on x^i, the system is *translationally invariant*. The famous example is the Lagrangian of a point particle of mass m in euclidean space:

$$L = \frac{m}{2}\dot{\mathbf{x}}^2. \tag{6.35}$$

If the indices are fully contracted with each other, the theory is *rotationally invariant*. In the first case, the system exhibits conservation of momentum, in the second case of angular momentum, as we now demonstrate.

Spatial Displacements

Under a spatial translation, the vector x^i changes as follows

$$x'^i = x^i + \epsilon^i, \tag{6.36}$$

where ϵ^i are small numbers. They give directly the infinitesimal translations of a particle path:

$$\delta_s x^i(t) = \epsilon^i \tag{6.37}$$

Under these, the Lagrangian changes by

$$\begin{aligned} \delta_s L &= L(x'^i(t), \dot x'^i(t), t) - L(x^i(t), \dot x^i(t), t) \\ &= \frac{\partial L}{\partial x^i}\delta_s x^i = \frac{\partial L}{\partial x^i}\epsilon^i = 0. \end{aligned} \tag{6.38}$$

By assumption, the Lagrangian is independent of x^i, so that the right-hand side vanishes. This is to be compared with the symmetry variation of the Lagrangian around the classical orbit, calculated via the chain rule with the help of the Euler-Lagrange equation:

$$\begin{aligned}\delta_{\rm s} L &= \left(\frac{\partial L}{\partial x^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i}\right)\delta_{\rm s} x^i + \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}^i}\delta_{\rm s} x^i\right] \\ &= \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}^i}\right]\epsilon^i \end{aligned} \tag{6.39}$$

From this we extract the conserved Noether charges

$$p^i = \frac{\partial L}{\partial \dot{x}^i}. \tag{6.40}$$

They are simply the canonical momenta of the system.

Rotations

Under rotations, the vector x^i changes as follows

$$x'^i = R^i{}_j x^j \tag{6.41}$$

where $R^i{}_j$ is a 3×3 rotation matrix. Infinitesimally, this can be written as

$$R^i{}_j = \delta^i{}_j - \varphi_k \epsilon_{kij} \tag{6.42}$$

where $\varphi_k = \hat{\varphi}_k \varphi$ is an infinitesimal rotation vector. The infinitesimal rotation of a particle path is

$$\delta_{\rm s} x^i(t) = x'^i(t) - x^i(t) = -\varphi^k \epsilon_{kij} x^j(\tau). \tag{6.43}$$

Under it, the Lagrangian changes by

$$\begin{aligned}\delta_{\rm s} L &= L(x'^i(t), \dot{x}'^i(t), t) - L(x^i(t), \dot{x}^i(t), t) \\ &= \frac{\partial L}{\partial x^i}\delta_{\rm s} x^i + \frac{\partial L}{\partial \dot{x}^i}\delta_{\rm s}\dot{x}^i \end{aligned} \tag{6.44}$$

It is useful to introduce the antisymmetric infinitesimal rotation tensor

$$\varphi_{ij} \equiv \varphi_k \epsilon_{kij}, \tag{6.45}$$

and write

$$\delta_{\rm s} x^i = -\varphi_{ij} x^j. \tag{6.46}$$

Then

$$\delta_{\rm s} L = -\left(\frac{\partial L}{\partial x^i} x^j + \frac{\partial L}{\partial \dot{x}^i}\dot{x}^j\right)\varphi_{ij} = 0. \tag{6.47}$$

The right-hand side vanishes since φ_{ij} is antisymmetric and L depends only on the rotational invariants $\mathbf{x}^2, \dot{\mathbf{x}}^2, \mathbf{x}\cdot\dot{\mathbf{x}}$ and powers thereof, by assumption. Hence, rotations are symmetry transformation.

We now calculate the symmetry variation of the Lagrangian via the chain rule with the help of the Euler-Lagrange and find:

$$\begin{aligned}\delta_{\rm s}L &= \left(\frac{\partial L}{\partial x^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i}\right)\delta_{\rm s}x^i + \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}^i}\delta_{\rm s}x^i\right] \\ &= -\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}^i}x^j\right]\varphi_{ij} = \frac{1}{2}\varphi_{ij}\frac{d}{dt}\left[x_i\frac{\partial L}{\partial \dot{x}^j} - (i \leftrightarrow j)\right] = 0. \end{aligned} \tag{6.48}$$

Equating this with (6.47) we obtain the conserved Noether charges

$$L^{ij} = x^i\frac{\partial L}{\partial \dot{x}^j} - x^j\frac{\partial L}{\partial \dot{x}^i} \equiv x^ip^j - x^jp^i. \tag{6.49}$$

They are the usual angular momenta.

Had we worked with the original rotation angles φ^k, we would have found them in the more common form:

$$L_k = \frac{1}{2}\epsilon_{kij}L^{ij} = (\mathbf{x}\times\mathbf{p})^k. \tag{6.50}$$

6.3.1 Center-of-Mass Theorem

Consider now the transformations corresponding to a uniform motion of the coordinate system. We shall study the behavior of a set of free massive point particles in euclidean space described by the Lagrangian

$$L = \sum_n \frac{m_n}{2}\dot{\mathbf{x}}^2. \tag{6.51}$$

Under Galilei transformations, the spatial coordinates and time are changes as follows:

$$\begin{aligned} x'^i(t) &= x^i(t) - v^it \\ t' &= t. \end{aligned} \tag{6.52}$$

where v^i is the relative velocity v. The symmetry variations are

$$\delta_{\rm s}x^i(t) = x'^i(t) - x^i(t) = -v^it. \tag{6.53}$$

The Lagrangian changes by

$$\delta_{\rm s}L = L(x^i - v^it, \dot{x}^i - v^i) - L(x^i, \dot{x}^i). \tag{6.54}$$

Inserting the explicit form (6.51), we obtain

$$\delta_{\rm s}L = \sum_n \frac{m_n}{2}\left[(\dot{x}_n^i - v^i)^2 - (\dot{x}_n{}^i)^2\right]. \tag{6.55}$$

This can be written as a total time derivative:

$$\delta_{\rm s} L = \frac{d}{dt}\Lambda = \frac{d}{dt}\sum_n m_n \left[-\dot{x}^i_n v^i + \frac{v^2}{2}t\right] \tag{6.56}$$

proving that Galilei transformations are symmetry transformation in the Noether sense. For infinitesimal velocities v^i, the second term can be ignored. Calculating $\delta_{\rm s}$ once more via the chain rule with the help of the Euler-Lagrange equations, and equating the result with (6.56), we find the conserved Noether charge

$$\begin{aligned} Q &= \sum_n \frac{\partial L}{\partial \dot{x}^i}\delta_{\rm s} x^i - \Lambda \\ &= \left(-\sum_n m_n \dot{x}^i_n t + \sum_n m_n x^i_n\right) v^i. \end{aligned} \tag{6.57}$$

Since the direction of the velocity v^i is arbitrary, each component

$$N^i = -\sum_n m_n \dot{x}^i t + \sum_n m_n {x_n}^i \tag{6.58}$$

is a constant of motion. This is the well-known *center-of-mass theorem.*[2] Indeed, introducing the center-of-mass coordinates

$$x^i_{\rm CM} \equiv \frac{\sum_n m_n {x_n}^i}{\sum_n m_n} \tag{6.59}$$

and velocities

$$v^i_{\rm CM} = \frac{\sum_n m_n {\dot{x}_n}^i}{\sum_n m_n} \tag{6.60}$$

the conserved charge (6.58) can be written as

$$N^i = \sum_n m_n(-v^i_{\rm CM} t + x^i_{\rm CM}), \tag{6.61}$$

so that the constancy of N^i implies that the center-of-mass moves with uniform velocity according to the law

$$x^i_{\rm CM}(t) = x^i_{0\,\rm CM} + v^i_{\rm CM} t, \tag{6.62}$$

where

$$x^i_{0\,\rm CM} = \frac{N^i}{\sum_n m_n}, \tag{6.63}$$

is the position of the center of mass at $t = 0$.

It is interesting to note that in non-relativistic physics, the center of mass theorem is a consequence of momentum conservation since momentum ≡ mass × velocity. In relativistic physics, this is no longer true.

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[2] See S. Coleman and J.H. Van Vleck, Phys. Rev. **171**, 1370 (1968).

6.3.2 Conservation Laws from Lorentz Invariance

In relativistic physics, particle orbits are described by functions in spacetime

$$x^\mu(\tau) \tag{6.64}$$

where τ is an arbitrary Lorentz-invariant parameter, and action are specified as integrals over τ:

$$\mathcal{A} = \int d\tau L\left(x^\mu(\tau), x'^\mu(\tau), \tau\right), \tag{6.65}$$

where $x'^\mu(\tau)$ denotes the derivative with respect to the parameter τ. If the Lagrangian depends only on invariant scalar products $x^\mu x_\mu, x^\mu \dot{x}_\mu, x'^\mu \dot{x}'_\mu$, then it is invariant under Lorentz transformations

$$x^\mu \to x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{6.66}$$

where $\Lambda^\mu{}_\nu$ is a 4×4 matrix satisfying

$$\Lambda g \Lambda^T = g, \tag{6.67}$$

with the Minkowski metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}. \tag{6.68}$$

For a free massive point particle in spacetime, the Lagrangian is

$$L(x'(\tau)) = -Mc\sqrt{g_{\mu\nu} x'^\mu x'^\nu}. \tag{6.69}$$

It is reparametrization invariant under $\tau \to f(\tau)$, with an arbitrary function $f(\tau)$. Under translations

$$\delta_s x^\mu(\tau) = x^\mu(\tau) - \epsilon^\mu(\tau), \tag{6.70}$$

the Lagrangian is obviously invariant satisfying , $\delta_s \mathcal{L}$. Calculating this variation once more via the chain rule with the help of the Euler-Lagrange equations, we find

$$\begin{aligned} 0 &= \int_{\tau_\mu}^{\tau_\nu} d\tau \left(\frac{\partial L}{\partial x^\mu} \delta_s x^\mu + \frac{\partial L}{\partial x'^\mu} \delta_s x'^\mu \right) \\ &= -\epsilon^\mu \int_{\tau_\mu}^{\tau_\nu} d\tau \frac{d}{d\tau} \left(\frac{\partial L}{\partial x'^\mu} \right). \end{aligned} \tag{6.71}$$

From this we obtain the Noether charges

$$p_\mu \equiv -\frac{\partial L}{\partial x'^\mu} = Mc \frac{x'_\mu(\tau)}{\sqrt{g_{\mu\nu} x'^\mu x'^\nu}} = Mcu^\mu, \tag{6.72}$$

which satisfy the conservation law

$$\frac{d}{d\tau}p_\mu(t) = 0. \tag{6.73}$$

They are the conserved four-momenta of a free relativistic particle. The quantity

$$u^\mu \equiv \frac{x'^\mu}{\sqrt{g_{\mu\nu}x'^\mu x'^\nu}} \tag{6.74}$$

is the dimensionless relativistic four-velocity of the particle. It has the property $u^\mu u_\mu = 1$ and is reparametrization invariant. By choosing for τ the physical time $t = x^0/c$, we can express u^μ in terms of the physical velocities $v^i = dx^i/dt$ as

$$u^\mu = \gamma(1, v^i/c), \qquad \text{with} \qquad \gamma \equiv \sqrt{1 - v^2/c^2}. \tag{6.75}$$

Note the minus sign in the definition of (6.72) of the canonical momentum with respect to the nonrelativistic case. It is necessary to write Eq. (6.72) covariantly. The derivative with respect to x'^μ transforms like a covariant vector with a subscript μ, whereas the physical momenta are p^μ.

For small Lorentz transformations near the identity we write

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \omega^\mu{}_\nu \tag{6.76}$$

where

$$\omega^\mu{}_\nu = g^{\mu\lambda}\omega_{\lambda\nu} \tag{6.77}$$

is an arbitrary infinitesimal antisymmetric matrix. An infinitesimal Lorentz transformation of the particle path is

$$\begin{aligned} \delta_{\rm s} x^\mu(\tau) &= x'^\mu(\tau) - x^\mu(\tau) & (6.78)\\ &= \omega^\mu{}_\nu x^\nu(\tau). & (6.79) \end{aligned}$$

Under it, the symmetry variation of a Lorentz-invariant Lagrangian vanishes:

$$\delta_{\rm s} L = \left(\frac{\partial L}{\partial x^\mu}x^\nu + \frac{\partial L}{\partial x'^\mu}x'^\nu\right)\omega^\mu{}_\nu = 0 \tag{6.80}$$

This is to be compared with the symmetry variation of the Lagrangian calculated via the chain rule with the help of the Euler-Lagrange equation

$$\begin{aligned} \delta_{\rm s} L &= \left(\frac{\partial L}{\partial x^\mu} - \frac{d}{d\tau}\frac{\partial L}{\partial x'^\mu}\right)\delta_{\rm s} x^\mu + \frac{d}{d\tau}\left[\frac{\partial L}{\partial x'^\mu}\delta_{\rm s} x^\mu\right] \\ &= \frac{d}{d\tau}\left[\frac{\partial L}{\partial x'^\mu}x'^\nu\right]\omega^\mu{}_\nu \\ &= \frac{1}{2}\omega_\mu{}^\nu \frac{d}{d\tau}\left(x^\mu\frac{\partial L}{\partial x'_\nu} - x^\nu\frac{\partial L}{\partial x'_\mu}\right). \end{aligned} \tag{6.81}$$

By equating this with (6.80) we obtain the conserved Noether charges [containing again a minus sign as in (6.72)]

$$L^{\mu\nu} = -x^\mu \frac{\partial L}{\partial x'_\nu} + x^\nu \frac{\partial L}{\partial x'_\mu} = x^\mu p^\nu - x^\nu p^\mu. \tag{6.82}$$

They are the four-dimensional generalizations of the angular momenta. The quantities L^{ij} coincide with the earlier-introduced angular momenta (6.49). The conserved components

$$L^{0i} = x^0 p^i - x^i p^0 \equiv M_i \tag{6.83}$$

yield the relativistic generalization of (6.58):

$$M_i = \text{const.} \tag{6.84}$$

6.4 Generating the Symmetries

A mentioned in the introduction to this chapter, the relation between invariances and conservation laws has a second aspect. After quantization, the charge associated with the continuous symmetry transformation from which it was derived can be used to generate this symmetry transformation in the Hilbert space. Explicitly,

$$\delta_s \hat{q} = -i\epsilon[\hat{Q}, \hat{q}(t)]. \tag{6.85}$$

The charge derived in Section 7.2 from the invariance of the system under time displacement is the most famous example for this property. The charge (6.29) is by definition the *Hamiltonian*,

$$Q \equiv H,$$

whose operator generates infinitesimal time displacements by the *Heisenberg equation of motion*:

$$\dot{\hat{q}}(t) = -i[\hat{H}, \hat{q}(t)]. \tag{6.86}$$

This equation is obviously the same as (6.85).

To quantize the system canonically, we may assume the Lagrangian to have the standard form

$$L(q, \dot{q}) = \frac{M}{2}\dot{q}^2 - V(q), \tag{6.87}$$

so that the *Hamiltonian operator* becomes, with the canonical momentum $p \equiv \dot{q}$:

$$\hat{H} = \frac{\hat{p}^2}{2M} + V(\hat{q}). \tag{6.88}$$

Equation (6.86) is then a direct consequence of the canonical commutation rules

$$[p(t), q(t)] = -i, \quad [p(t), p(t)] = 0, \quad [q(t), q(t)] = -i. \tag{6.89}$$

The charges (6.40) derived Section 7.3 from translational symmetry are another famous example. After quantization, the commutation rule (6.85) becomes, with (6.37),

$$\epsilon^j = i\epsilon^i[\hat{p}^i, \hat{x}^j(t)]. \tag{6.90}$$

This coincides with one of the canonical commutation relations (here it appears only for time-independent momenta, since the system is translationally invariant).

The relativistic charges (6.72) of spacetime generate translations via

$$\delta_{\rm s} x^\mu = \epsilon^\mu = -i\epsilon^\nu[\hat{p}_\nu, \hat{x}^\mu(\tau)]. \tag{6.91}$$

in agreement with the relativistic canonical commutation rules (3.33).

Similarly we find that the quantized versions of the conserved charges L_i in Eq. (6.50) generate infinitesimal rotations:

$$\delta_{\rm s} x^j = -\varphi^i\epsilon_{ijk}\hat{x}^k(t) = i\varphi^i[\hat{L}_i, \hat{x}^j(t)], \tag{6.92}$$

while the quantized conserved charges N^i of Eq. (6.58) generate infinitesimal Galilei transformations, and that the charges M_i of Eq. (6.83) generate pure Lorentz transformations:

$$\begin{aligned} \delta_{\rm s} x^j &= \epsilon_i x^0 = i\epsilon_i[M_i, x^j] \\ \delta_{\rm s} x^0 &= \epsilon_i x^i = i\epsilon_i[M_i, x^0]. \end{aligned} \tag{6.93}$$

Since the quantized charges generate the symmetry transformation, they form a *representation* of the generators of the symmetry group. They therefore have the same commutation rules among each other as the generators of the symmetry group. The charges (6.50) associated with rotations, for example, have the commutation rules

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk}\hat{L}_j, \tag{6.94}$$

which are the same as those between the 3 × 3 generators of the three-dimensional rotations $(L_i)_{jk} = -i\epsilon_{ijk}$.

The quantized charges of the generators (6.82) of the Lorentz group satisfy the commutation rules of the 4 × 4 generators (3.82):

$$[\hat{L}^{\mu\nu}, \hat{L}^{\mu\lambda}] = -ig^{\mu\mu}\hat{L}^{\nu\lambda}. \tag{6.95}$$

This follows directly from the canonical commutation rules (6.91) [i.e., (3.33)].

6.5 Field Theory

A similar relation between continuous symmetries and constants of motion holds in field theories.

6.5.1 Continuous Symmetry and Conserved Currents

If

$$\mathcal{A} = \int d^4x \mathcal{L}(\varphi, \partial\varphi, x) \tag{6.96}$$

is the action of an arbitrary field $\varphi(x)$ and if

$$\delta_s \mathcal{L}(x) = \epsilon\Delta(\varphi, \partial\varphi, x) \tag{6.97}$$

changes the action $\mathcal{L}$ merely by a surface term

$$\delta_s \mathcal{L} = \epsilon \int d^4x \partial_\mu \Lambda^\mu \tag{6.98}$$

or equivalently, if the Lagrangian density $\mathcal{L}$ changes by a total derivative

$$\delta_s \mathcal{L} = \epsilon \partial_\mu \Lambda^\mu. \tag{6.99}$$

Then $\delta_s \mathcal{L}$ is called a *symmetry transformation.*

Given such a symmetry transformation we can find a current four-vector

$$j^\mu = \frac{\partial L}{\partial \partial_\mu \varphi} \Delta - \Lambda^\mu \tag{6.100}$$

that has no four-divergence

$$\partial_\mu j^\mu(x) = 0. \tag{6.101}$$

This is called a *local conservation law.*

Assuming all fields to vanish at spatial infinity, this implies a *global conservation law* for the charge associated with j^μ:

$$Q(t) = \int d^3x j^0(\mathbf{x}, t). \tag{6.102}$$

Writing

$$\frac{d}{dt} Q(t) = \int d^3x \partial_0 j^0(\mathbf{x}, t) \tag{6.103}$$

we add to the integral on the right-hand side a vanishing integral over a total three-divergence, and find

$$\frac{d}{dt} Q(t) = \int d^3x \partial_0 j^0(\mathbf{x}, t) = \int d^3x [\partial_0 j^0(\mathbf{x}, t) + \partial_i j^i(\mathbf{x}, t)] = 0 \tag{6.104}$$

Thus the charge is independent of time:

$$\frac{d}{dt} Q(t) = 0. \tag{6.105}$$

The proof of the local conservation law (6.101) is just as easy as for the mechanical action (6.1). We calculate the symmetry variation of $\mathcal{L}$ under the symmetry transformation in a similar way as in Eq. (6.11), and find

$$\begin{aligned} \delta_{\rm s}\mathcal{L} &= \left(\frac{\partial \mathcal{L}}{\partial \varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi}\right)\delta_{\rm s}\varphi + \partial_\mu\left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi}\delta_{\rm s}\varphi\right) \\ &= \epsilon\left(\frac{\partial \mathcal{L}}{\partial \varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi}\right)\Delta + \partial_\mu\left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi}\Delta\right). \end{aligned} \tag{6.106}$$

Then we invoke the Euler-Lagrange equation to remove the first term. Equating the second term with (6.99) we obtain

$$\partial_\mu j^\mu \equiv \partial_\mu\left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi}\Delta - \Lambda^\mu\right) = 0. \tag{6.107}$$

The relation between continuous symmetries and conservation is called *Noether's theorem.*[3]

6.5.2 Alternative Derivation

There is again an alternative derivative of the conserved current analogous to Eqs. (6.15)–(6.21). It is based on a variation of the fields under symmetry transformation whose parameter ϵ is made artificially space independent $\epsilon(x)$; extending (6.15):

$$\delta_{\rm s}^x\varphi(t) = \epsilon(x)\Delta(\varphi(x), \partial_\mu\varphi(x), x). \tag{6.108}$$

As before in Eq. (6.17), let us introduce a Lagrangian density for a field

$$\varphi^\epsilon(t) \equiv \varphi(t) + \delta_{\rm s}^x\varphi(t) \tag{6.109}$$

which differs from a classical field by a symmetry variation (6.108). This can be expanded as:

$$L^\epsilon \equiv L(\varphi^\epsilon(t), \partial\varphi^\epsilon(t)). \tag{6.110}$$

Then the variation of the action corresponding to (6.18) is

$$\delta_{\rm s}^x\mathcal{A} = \int dx \left\{\left[\frac{\partial \mathcal{L}^\epsilon}{\partial \epsilon(x)} - \partial_\mu \frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)}\right]\delta\epsilon(x) + \partial_\mu\left[\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)}\delta\epsilon(x)\right]\right\}. \tag{6.111}$$

From this we obtain the Euler-Lagrange-like equation

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \epsilon(x)} - \partial_\mu \frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon(x)} = 0. \tag{6.112}$$

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[3] Elly Noether, Nachr. d. vgl. Ges. d. Wiss. Göttingen, Math-Phys. Klasse, 235 (1918; See also Bessel-Hagen, Math. Ann. **84**, 258 (1926);
L. Rosenfeld, Me. Acad. Roy. Belg. **18**, 2 (1938);
F. Belinfante, Physica **6**, 887 (1939).

By assumption, the action was a pure surface term under x-independent transformations, implying that

$$\frac{\partial \mathcal{L}^{\epsilon}}{\partial \epsilon(x)} = \partial_{\mu} \Lambda^{\mu}. \tag{6.113}$$

Together with (6.112) we see that

$$j^{\mu} = \frac{\partial \delta_{\rm s}^{x} \mathcal{L}}{\partial \partial_{\mu} \epsilon(x)} - \Lambda^{\mu} \tag{6.114}$$

has no four-divergence. By the chain rule of differentiation

$$\delta_{\rm s}^{t} \mathcal{L} = \frac{\partial \mathcal{L}(x)}{\partial \varphi} \epsilon \Delta + \frac{\partial \mathcal{L}}{\partial \partial_{\nu} \varphi} \partial_{\nu} \epsilon \Delta, \tag{6.115}$$

so that

$$\frac{\partial \mathcal{L}^{\epsilon}}{\partial \partial_{\mu} \epsilon(x)} = \frac{\partial \mathcal{L}}{\partial \partial_{\mu} \varphi} \, \Delta(\varphi, \partial \varphi, x), \tag{6.116}$$

i.e., the current (6.114) coincide with (6.100).

Note that (6.116) can also be written as

$$\frac{\partial \mathcal{L}^{\epsilon}}{\partial \partial_{\mu} \epsilon} = \frac{\partial \mathcal{L}}{\partial \partial_{\mu} \varphi} \frac{\partial \delta_{\rm s}^{x} \varphi}{\partial \epsilon} \tag{6.117}$$

6.6 Canonical Energy Momentum Tensor

As an important example for the field theoretic version of the theorem consider the usual case that the Lagrangian density does not depend explicitly on the space-time coordinates x:

$$\mathcal{L} = \mathcal{L}(\varphi, \partial \varphi). \tag{6.118}$$

We then perform a translation along an arbitrary direction $\nu = 0, 1, 2, 3$ of spacetime

$$x'^{\mu} = x^{\mu} - \epsilon^{\mu}, \tag{6.119}$$

under which field $\varphi(x)$ transforms as

$$\varphi'(x') = \varphi(x). \tag{6.120}$$

This equation expresses the fact that at the same absolute point in space and time, which in one coordinate term is labeled by the coordinates x^{μ} and in the other by x'^{μ}, the field has the same value.

Under an infinitesimal translation of the field configuration coordinate the Lagrangian density undergoes the following symmetry variation

$$\begin{aligned} \delta_{\rm s} \mathcal{L} &\equiv \mathcal{L}(\varphi'(x), \partial \varphi'(x)) - \mathcal{L}(\varphi(x), \partial \varphi(x)) \\ &= \frac{\partial \mathcal{L}}{\partial \varphi(x)} \delta_{\rm s} \varphi(x) + \frac{\partial \mathcal{L}}{\partial \partial_{\mu} \varphi} \partial_{\mu} \delta_{\rm s} \varphi(x), \end{aligned} \tag{6.121}$$

where

$$\delta_s\varphi(x) = \varphi'(x) - \varphi(x) \tag{6.122}$$

is the symmetry variation of the fields. For the particular transformation (6.120), the symmetry variation becomes simply

$$\delta_s\varphi(x) = \epsilon^\nu \partial_\nu \varphi(x). \tag{6.123}$$

The Lagrangian density (6.118) changes by

$$\delta_s\mathcal{L}(x) = \epsilon^\nu \partial_\nu \mathcal{L}(x). \tag{6.124}$$

Hence the requirement (6.98) is satisfied and $\delta_s\varphi(x)$ is a symmetry transformation. The function Λ happens to coincide with the Lagrangian density

$$\Lambda = \mathcal{L}. \tag{6.125}$$

We can now define a set of currents $j_\nu{}^\mu$, one for each ϵ^ν, which in the particular case at hand are denoted by $\Theta_\nu{}^\mu$,

$$\Theta_\nu{}^\mu = \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_\nu\varphi - \delta_\nu{}^\mu\mathcal{L}. \tag{6.126}$$

They have no four divergence

$$\partial_\mu\Theta_\nu{}^\mu(x) = 0. \tag{6.127}$$

As a consequence, the *total four momentum* of the system defined by

$$P^\mu = \int d^3x \Theta^{\mu 0}(x) \tag{6.128}$$

is independent of time.

The alternative derivation of the currents goes as follows. Introducing

$$\delta_s^x\varphi(x) = \epsilon^\nu(x)\partial_\nu\varphi(x) \tag{6.129}$$

we see that

$$\delta_s^x\varphi(x) = \varphi^\nu(x)\partial_\nu\varphi(x). \tag{6.130}$$

On the other hand, the chain rule of differentiation yields

$$\delta_s^x\mathcal{L} \;=\; \frac{\partial\mathcal{L}}{\partial\varphi(x)}\epsilon^\nu(x)\partial_\nu\varphi(x) + \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi(x)}\left\{[\partial_\mu\epsilon^\nu(x)]\partial_\nu\varphi + \epsilon^\nu\partial_\mu\partial_\nu\varphi(x)\right\}. \tag{6.131}$$

Hence

$$\frac{\partial\mathcal{L}^\epsilon}{\partial\partial_\mu\epsilon^\nu(x)} = \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_\nu\varphi \tag{6.132}$$

and we obtain again the energy-momentum tensor (6.126).

Note that (6.132) can also be written as

$$\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \epsilon^\nu(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\mu \varphi} \frac{\partial \delta_{\rm s}^x \varphi}{\partial \epsilon^\nu(x)} \tag{6.133}$$

Since ν is a contravariant vector index, the set of currents ${\Theta_\nu}^{\mu u}$ forms a Lorentz tensor called the *canonical energy momentum tensor*. The component

$${\Theta_0}^0 = \frac{\partial \mathcal{L}}{\partial \partial_0 \varphi} \partial_0 \varphi - \mathcal{L} \tag{6.134}$$

is recognized to be the Hamiltonian density in the canonical formalism.

6.6.1 Electromagnetism

As a an important physical application of the field theoretic Noether theorem, consider the free electromagnetic field with the action

$$\mathcal{L} = -\frac{1}{4c} F_{\lambda\kappa} F^{\lambda\kappa}, \tag{6.135}$$

where F_κ are the field strength $F_{\lambda\kappa} \equiv \partial_\lambda A_\kappa - \partial_\kappa A_\lambda$. Under a translation in space and time from x^μ to $x^\mu - \epsilon \delta_\nu^\mu$, the vector potential undergoes a similar change as in (6.120):

$$A'^\mu(x') = \Lambda^\mu(x). \tag{6.136}$$

As before, this equation expresses the fact that at the same absolute space time point, which in the two coordinate frames is labeled once by x' and once by x, the field components have the same numerical values. The equation transformation law (6.136) can be rewritten in an infinitesimal form as

$$\begin{aligned} \delta_{\rm s} A^\lambda(x^\mu) &\equiv A'^\lambda(x^\mu) - A^\lambda(x^\mu) \\ &= A'^\lambda(x'^\mu + \epsilon {\delta_\nu}^\mu) - A^\lambda(x^\mu) &(6.137)\\ &= \epsilon \partial_\nu A^\lambda(x^\mu). &(6.138)\end{aligned}$$

Under it, the field tensor changes as follows

$$\delta_{\rm s} F^{\lambda\kappa} = \epsilon \partial_\nu F^{\lambda\kappa}, \tag{6.139}$$

so that the Lagrangian density is a total four divergence:

$$\delta_{\rm s} \mathcal{L} = -\epsilon \frac{1}{2c} F_{\lambda\kappa} \partial_\nu F^{\lambda\kappa} = \epsilon \partial_\nu \mathcal{L} \tag{6.140}$$

Thus, the spacetime translations (6.138) are symmetry transformation, and the currents

$${\Theta_\nu}^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu A^\lambda} \partial_\nu A^\lambda - {\delta_\nu}^\mu \mathcal{L} \tag{6.141}$$

are conserved:

$$\partial_\mu \Theta_\nu{}^\mu(x) = 0. \tag{6.142}$$

Using $\partial\mathcal{L}/\partial\partial_\mu A^\lambda = -F^\mu{}_\lambda$, this becomes more explicitly

$$\Theta_\nu{}^\mu = -\frac{1}{c}\left(F^\mu_\lambda \partial_\nu A^\lambda - \frac{1}{4}\delta_\nu{}^\mu F^{\lambda\kappa}F_{\lambda\kappa}\right). \tag{6.143}$$

This is the *canonical energy momentum tensor* of the electromagnetic field.

6.6.2 Dirac Field

We now turn to the Dirac field. For the calculation of conserved currents it is important to use, instead of (3.447) and (5.205), a hermitian Dirac Lagrangian density

$$\mathcal{A} = \int d^4x \mathcal{L}(x) = \int d^4x \bar{\psi}(x)(i\gamma^\mu \overleftrightarrow{\partial}_\mu - M)\psi(x), \tag{6.144}$$

Under spacetime translations

$$x'^\mu = x^\mu - \epsilon^\mu, \tag{6.145}$$

the Dirac field transforms in the same way as the previous scalar and vector fields:

$$\psi'(x') = \psi(x), \tag{6.146}$$

or infinitesimally:

$$\delta_s \psi(x) = \epsilon^\mu \partial_\mu \psi(x). \tag{6.147}$$

The same thing is true for the Lagrangian density, where

$$\mathcal{L}'(x') = \mathcal{L}(x), \tag{6.148}$$

and

$$\delta_s \mathcal{L}(x) = \epsilon^\mu \partial_\mu \mathcal{L}(x). \tag{6.149}$$

Thus we obtain the Noether current

$$\Theta_\nu{}^\mu = \frac{\partial\mathcal{L}}{\partial\partial_\mu\psi^\lambda}\partial_\nu\psi^\lambda + \mathrm{cc} - \delta_\nu{}^\mu\mathcal{L} \tag{6.150}$$

with the local conservation law

$$\partial_\mu \Theta_\nu{}^\mu(x) = 0. \tag{6.151}$$

From (6.144) we see that

$$\frac{\partial\mathcal{L}}{\partial\partial_\mu\psi^\lambda} = \frac{1}{2}\bar{\psi}\gamma^\mu \tag{6.152}$$

so that we obtain the *canonical energy momentum tensor* of the Dirac field:

$$\Theta_\nu{}^\mu = \frac{1}{2}\bar{\psi}\gamma^\mu\partial_\nu\psi^\lambda + \mathrm{cc} - \delta_\nu{}^\mu\mathcal{L} \tag{6.153}$$

6.7 Angular Momentum

Let us now turn to angular momentum in field theory. Consider first the case of a scalar field $\varphi(\dot{x})$. Under a rotation of the coordinates,

$$x'^i = R^i{}_j x^j \tag{6.154}$$

the field does not change, if considered at the same space point, i.e.,

$$\varphi'(x'^i) = \varphi(x^i). \tag{6.155}$$

The symmetry variation is:

$$\delta_s \varphi(x) = \varphi'(x) - \varphi(x). \tag{6.156}$$

Using the infinitesimal form (6.46) of (6.154),

$$\delta x^i = -\varphi_{ij} x^j, \tag{6.157}$$

we see that

$$\begin{aligned} \delta_s \varphi(x) &= \varphi'(x^0, x'^i - \delta x^i) - \varphi(x) \\ &= \partial_i \varphi(x) x^j \varphi_{ij}. \end{aligned} \tag{6.158}$$

Suppose we are dealing with a rotationally Lorentz-invariant Lagrangian density which has no explicit x-dependence:

$$\mathcal{L} = \mathcal{L}(\varphi(x), \partial\varphi(x)). \tag{6.159}$$

Then the symmetry variation is

$$\begin{aligned} \delta_s \mathcal{L} &= \mathcal{L}(\varphi'(x), \partial\varphi'(x)) - \varphi(\varphi(x), \partial\varphi(x)) \\ &= \frac{\partial \mathcal{L}}{\partial \varphi(x)} \delta_s \varphi(x) + \frac{\partial \varphi}{\partial \partial \varphi(x)} \partial_\mu \delta_s \varphi(x) \end{aligned} \tag{6.160}$$

For a Lorentz-invariant $\mathcal{L}$, the derivative $\partial\mathcal{L}/\partial\partial_\mu\varphi$ is a vector proportional to $\partial_\mu\varphi$. More explicitly, Eq. (6.158) reads

$$\begin{aligned} \delta_s \mathcal{L} &= \left[\frac{\partial \mathcal{L}}{\partial \varphi} \partial_i \varphi x^j + \frac{\partial \mathcal{L}}{\partial_\mu \varphi} \partial_\mu (\partial_i \mathcal{L} x^j) \right] \varphi_{ij} \\ &= \left[(\partial_i \mathcal{L}) x^j + \frac{\partial \mathcal{L}}{\partial \partial_j \varphi} \partial_i \varphi \right] \varphi_{ij} = \partial_i \left(\mathcal{L} x^j \varphi_{ij} \right) \end{aligned} \tag{6.161}$$

The right-hand side is a total derivative. In arriving at this result, the antisymmetry of φ_{ij} has been used twice: once in order to drop the second term in the brackets, which is possible since $\partial\mathcal{L}/\partial\partial_i\varphi$ is proportional to $\partial_i\varphi$, as a consequence of the assumed rotational invariance of $\mathcal{L}$,[4] and once, in order to pull x^j inside the last parentheses.

Calculating $\delta_{\rm s}\mathcal{L}$ once more using the Euler-Lagrange equations gives

$$\begin{aligned}\delta_{\rm s}\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\mathcal{L}}\delta_{\rm s}\varphi + \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_\mu\delta_{\rm s}\varphi \\ &= \left(\frac{\partial\mathcal{L}}{\partial\varphi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\right)\delta_{\rm s}\varphi + \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\delta_{\rm s}\varphi\right) \\ &= \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_i\varphi\, x^j\right)\varphi_{ij}.\end{aligned} \tag{6.162}$$

Thus the Noether charges

$$L^{ij,\mu} = \left(\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_i\varphi x^j - \delta_i{}^\mu\mathcal{L}\, x^j\right) - (i \leftrightarrow j) \tag{6.163}$$

have no four-divergence

$$\partial_\mu L^{ij,\mu} = 0. \tag{6.164}$$

The associated charges

$$L^{ij} = \int d^3x L^{ij,\mu} \tag{6.165}$$

are called the *total angular momenta* of the field system. Remembering the canonical energy momentum tensor

$$\Theta_\nu{}^\mu = \frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}\partial_\nu\varphi - \delta_\nu{}^\mu\mathcal{L}, \tag{6.166}$$

we see that $L^{ij,\mu}$ can also be rewritten as

$$L^{ij,\mu} = x^i\Theta^{j\mu} - x^j\Theta^{i\mu}. \tag{6.167}$$

6.8 Four-Dimensional Angular Momentum

A similar procedure applies to pure Lorentz transformations. An infinitesimal boost to a rapidity ζ^i produces a coordinate change

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu = x^\mu + \delta^\mu{}_i\zeta^i x^\nu + \delta^\mu{}_0\zeta^i x^i. \tag{6.168}$$

This can be written as

$$\delta x^\mu = \omega^\mu{}_\nu x^\nu, \tag{6.169}$$

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[4] Recall the similar argument after Eq. (6.47)

where

$$\begin{aligned} \omega_{ij} &= 0, \\ \omega_{0i} = -\omega_{i0} &= \zeta^i. \end{aligned} \tag{6.170}$$

With the tensor $\omega^\mu{}_\nu$, the restricted Lorentz transformations and the infinitesimal rotations can be treated on the same footing. The rotations have the form (6.169) for the particular choice

$$\begin{aligned} \omega_{ij} &= \varphi_{ij} = \epsilon_{ijk}\varphi^k \\ \omega_{0i} &= \omega_{i0} = 0. \end{aligned} \tag{6.171}$$

We can now identify the symmetry variations of the filed as being

$$\begin{aligned} \delta_s\varphi(x) &= \varphi'(x'^\mu - \delta x^\mu) - \varphi(x) \\ &= -\partial_\mu\varphi(x)x^\nu\omega^\mu{}_\nu. \end{aligned} \tag{6.172}$$

Just as in (6.161), the Lagrangian density transforms as the total derivative

$$\delta_s\varphi = -\partial_\mu(\mathcal{L}x^\nu)\omega^\mu{}_\nu \tag{6.173}$$

and we obtain the Noether currentss

$$L^{\mu\nu,\lambda} = -\left(\frac{\partial\mathcal{L}}{\partial\partial_\lambda\varphi}\partial^\lambda\varphi x^\nu - \delta^{\mu\lambda}\mathcal{L}x^\nu\right) - (\mu\leftrightarrow\nu) \tag{6.174}$$

The right-hand side can be expressed in terms of the canonical energy-momentum tensor (6.126) so that we find

$$\begin{aligned} L^{\mu\nu,\lambda} &= -\left(\frac{\partial\mathcal{L}}{\partial\partial_\lambda\varphi}\partial^\lambda\varphi x^\nu - \delta^{\mu\lambda}\mathcal{L}x^\nu\right) - (\mu\leftrightarrow\nu) \\ &= x^\mu\Theta^{\nu\lambda} - x^\nu\Theta^{\mu\lambda}. \end{aligned} \tag{6.175}$$

These currents have no four-divergence

$$\partial_\lambda L^{\mu\nu,\lambda} = 0. \tag{6.176}$$

The associated charges

$$L^{\mu\nu} \equiv \int d^3x L^{\mu\nu,0} \tag{6.177}$$

are independent of time.

For the particular form of $\omega_{\mu\nu}$ in (6.170), we find time independent components L^{i0}. The components L^{ij} coincide with the previously-derived angular momenta.

The constancy of L^{i0} is the relativistic version of the center-of-mass theorem (6.62). Indeed, since

$$L^{i0} = \int d^3x(x^i\Theta^{00} - x^0\Theta^{i0}), \tag{6.178}$$

we can then define the relativistic center of mass

$$x^i_{\rm CM} = \frac{\int d^3x \Theta^{00} x^i}{\int d^3x \Theta^{00}} \tag{6.179}$$

and the average velocity

$$v^i_{\rm CM} = c\frac{d^3x\Theta^{i0}}{\int d^3x\Theta^{00}} = c\frac{P^i}{P^0} \tag{6.180}$$

Since $\int d^3x\Theta^{i0} = P^i$ is the constant momentum of the system, also $v^i_{\rm CM}$ is a constant. Thus, the constancy of L^{0i} implies the center of mass to move with the constant velocity

$$x^i_{\rm CM}(t) = x^i_{0\rm CM} + v^i_{0\rm CM}t \tag{6.181}$$

with $x^i_{0\rm CM} = L^{0i}/P^0$.

The quantities $L^{\mu\nu}$ are referred to as four-dimensional orbital angular momenta.

It is important to point out that the vanishing divergence of $L^{\mu\nu,\lambda}$ makes $\Theta^{\nu\mu}$ symmetric:

$$\begin{aligned}\partial_\lambda L^{\mu\nu,\lambda} &= \partial_\lambda(x^\mu\Theta^{\nu\lambda} - x^\nu\Theta^{\mu\lambda}) \\ &= \Theta^{\nu\mu} - \Theta^{\nu\mu} = 0.\end{aligned} \tag{6.182}$$

Thus, translationally invariant field theories whose orbital angular momentum is conserved have always a symmetric canonical energy momentum tensor.

$$\Theta^{\mu\nu} = \Theta^{\nu\mu} \tag{6.183}$$

6.9 Spin Current

If the field $\varphi(x)$ is no longer a scalar but has several spatial components, then the derivation of the four-dimensional angular momentum becomes slightly more involved.

6.9.1 Electromagnetic Fields

Consider first the case of electromagnetism where the relevant field is the four-vector potential $A^\mu(x)$. When going to a new coordinate frame

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{6.184}$$

the vector field at the same point remains unchanged in absolute space-time. But since the components A^μ refer to two different basic vectors in the different frames, they must be transformed simultaneously with x^μ. Since $A^\mu(x)$ is a vector, it transforms as follows:

$$A'^\mu(x') = \Lambda^\mu{}_\nu A^\nu(x). \tag{6.185}$$

For an infinitesimal transformation

$$\delta_{\rm s} x^\mu = \omega^\mu{}_\nu x^\nu \tag{6.186}$$

this implies the symmetry variation

$$\begin{aligned}\delta_{\rm s} A^\mu(x) &= A'^\mu(x) - A^\mu(x) = A'^\mu(x-\delta x) - A^\mu(x)\\ &= \omega^\mu{}_\nu A^\nu(x) - \omega^\lambda{}_\nu x^\nu \partial_\lambda A^\mu.\end{aligned} \tag{6.187}$$

The first term is a *spin transformation*, the other an *orbital transformation.* This transformation can also be written in terms of the generators (3.61) and (3.61) of the Lorentz group as

$$\delta_{\rm s} A^\mu(x) = -i\omega^{\mu\nu} \hat{J}_{\mu\nu} A(x), \tag{6.188}$$

where

$$\hat{J}_{\mu\nu} = \hat{L}_{\mu\nu} + L_{\mu\nu} \tag{6.189}$$

is the operator of total four-dimensional angular momentum.

If the Lagrangian density involves only scalar combinations of four-vectors A^μ and if it has no explicit x-dependence, it changes under Lorentz transformations like a scalar field:

$$\mathcal{L}'(x') \equiv \mathcal{L}(A'(x'), \partial' A'(x')) = \mathcal{L}(A(x), \partial A(x)) \equiv \mathcal{L}(x). \tag{6.190}$$

Infinitesimally, this amounts to

$$\delta_{\rm s}\mathcal{L} = -(\partial_\mu \mathcal{L} x^\nu)\omega^\mu{}_\nu. \tag{6.191}$$

With the Lorentz transformations being symmetry transformation in the Noether sense, we calculate as in (6.163) the *current of total four-dimensional angular momentum*:

$$J^{\mu\nu,\lambda} = \frac{\partial\mathcal{L}}{\partial\partial_\lambda A_\mu} A^\nu - \left(\frac{\partial\mathcal{L}}{\partial\partial_\lambda A^\kappa}\partial^\mu A^\kappa x^\nu - \delta^{\mu\lambda}\mathcal{L}x^\nu\right) - (\mu \leftrightarrow \nu). \tag{6.192}$$

The last two terms have the same form as the current $L^{\mu\nu,\lambda}$ of the four-dimensional angular momentum of the scalar field. Here they are the *currents of the four-dimensional orbital angular momentum:*.

$$L^{\mu\nu,\lambda} = -\left(\frac{\partial\mathcal{L}}{\partial\partial_\lambda A^\kappa}\partial^\mu A^\kappa x^\nu - \delta^{\mu\lambda}\mathcal{L}x^\nu\right) - (\mu \leftrightarrow \nu). \tag{6.193}$$

Note that this current has the form

$$L^{\mu\nu,\lambda} = -i\frac{\partial\mathcal{L}}{\partial\partial_\lambda A^\kappa}\hat{L}^{\mu\nu} A^\kappa + \left[\delta^{\mu\lambda}\mathcal{L}x^\nu - (\mu \leftrightarrow \nu)\right]. \tag{6.194}$$

where $\hat{L}^{\mu\nu}$ are the differential operators of four-dimensional angular momentum (3.91).

Just as the scalar case (6.175), the currents (6.193) can be expressed in terms of the canonical energy momentum tensor as

$$L^{\mu\nu,\lambda} = x^\mu \Theta^{\nu\lambda} - x^\nu \Theta^{\mu\lambda}. \tag{6.195}$$

The first term in (6.192),

$$\Sigma^{\mu\nu,\lambda} = \left[\frac{\partial\mathcal{L}}{\partial\partial_\lambda A_\nu} A^\nu - (\mu \leftrightarrow \nu)\right], \tag{6.196}$$

is referred to as the *spin current*. It can be written in terms of the 4 × 4-generators (3.61) of the Lorentz group as

$$\Sigma^{\mu\nu,\lambda} = -i\frac{\partial\mathcal{L}}{\partial\partial_\lambda A^\kappa}(L^{\mu\nu})_{\kappa\sigma} A^\sigma. \tag{6.197}$$

The two currents together

$$J^{\mu\nu,\lambda}(x) \equiv \Sigma^{\mu\nu,\lambda}(x) + L^{\mu\nu,\lambda}(x) \tag{6.198}$$

are conserved, $\partial_\lambda J^{\mu\nu,\lambda}(x) = 0$. Individually, the terms are not conserved.

The total angular momentum is given by the charge

$$J^{\mu\nu} = \int d^3x J^{\mu\nu,0}(x). \tag{6.199}$$

It is a constant of motion. Using the conservation law of the energy momentum tensor we find, just as in (6.182), that the orbital angular momentum satisfies

$$\partial_\lambda L^{\mu\nu,\lambda}(x) = -\left[\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)\right]. \tag{6.200}$$

From this we find the divergence of the spin current

$$\partial_\lambda \Sigma^{\mu\nu,\lambda}(x) = -\left[\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)\right]. \tag{6.201}$$

For the charges associated with orbital and spin currents

$$L^{\mu\nu}(t) \equiv \int d^3x L^{\mu\nu,0}(x), \qquad \Sigma^{\mu\nu}(t) \equiv \int d^3x \Sigma^{\mu\nu,0}(x), \tag{6.202}$$

this implies the following time dependence:

$$\begin{aligned} \dot{L}^{\mu\nu}(t) &= -\int d^3x \left[\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)\right], \\ \dot{\Sigma}^{\mu\nu}(t) &= \int d^3x \left[\Theta^{\mu\nu}(x) - \Theta^{\nu\mu}(x)\right]. \end{aligned} \tag{6.203}$$

Fields with spin have always have a non-symmetric energy momentum tensor.

Then the current $J^{\mu\nu,\lambda}$ becomes

$$J^{\mu\nu,\lambda} = \left(\frac{\partial \delta_{\rm s}^x \mathcal{L}}{\partial \partial_\lambda \omega_{\mu\nu}(x)} - \delta^{\mu\lambda} \mathcal{L} x^\nu \right) - (\mu \leftrightarrow \nu) \tag{6.204}$$

By the chain rule of differentiation, the derivative with respect to $\partial, \omega_{\mu\nu}(x)$ can come only from field derivatives. For a scalar field

$$\frac{\partial \delta_{\rm s}^x \mathcal{L}}{\partial \partial_\lambda \omega_{\mu\nu}(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\lambda \varphi} \frac{\partial \delta_{\rm s}^x \varphi}{\partial \omega_{\mu\nu}(x)}, \tag{6.205}$$

and for a vector field

$$\frac{\partial \delta_{\rm s}^x \mathcal{L}}{\partial \partial_\lambda \omega_{\mu\nu}(x)} = \frac{\partial \mathcal{L}}{\partial \partial_\lambda A^\kappa} \frac{\partial \delta_{\rm s}^x A^\kappa}{\partial \omega_{\mu\nu}} \tag{6.206}$$

The alternative rule of calculating angular momenta is to introduce spacetime-dependent transformations

$$\delta^x x = \omega^\mu{}_\nu(x) x^\nu \tag{6.207}$$

under which the scalar fields transform as

$$\delta_{\rm s} \varphi = -\partial_\lambda \varphi \omega^\lambda{}_\nu(x) x^\nu \tag{6.208}$$

and the Lagrangian density as

$$\delta_{\rm s}^x \varphi = -\partial_\lambda \mathcal{L} \omega^\lambda{}_\nu(x) x^\nu = -\partial_\lambda (x^\nu \mathcal{L}) \omega^\lambda{}_\nu(x) \tag{6.209}$$

By separating spin and orbital transformations of $\delta_{\rm s}^x A^\kappa$ we find the two contributions $S^{\mu\nu,\lambda}$ and $L^{\mu\nu,\lambda}$ to the current $J^{\mu\nu,\lambda}$ of the total angular momentum, the latter receiving a contribution from the second term in (6.204).

6.9.2 Dirac Field

We now turn to the Dirac field. Under the Lorentz transformation (6.184), this transforms according to the law (3.47):

$$\psi(x) \xrightarrow{\Lambda} \psi'_\Lambda(x) = D(\Lambda) \psi(\Lambda^{-1} x). \tag{6.210}$$

For an infinitesimal Lorentz transformation

$$\Lambda_\mu{}^\nu = \delta_\mu{}^\nu + \omega_\mu{}^\nu, \tag{6.211}$$

the coordinates are changed by

$$\delta_{\rm s} x^\mu = \omega^\mu{}_\nu x^\nu \tag{6.212}$$

and the field has the symmetry variation [compare (3.476)]:

$$\begin{aligned} \delta_{\rm s} \psi(x) &= \psi'(x) - \psi(x) = D(\delta_\mu{}^\nu + \omega_\mu{}^\nu) \psi(x - \delta x) \\ &= -i \frac{1}{2} \omega_{\mu\nu} S^{\mu\nu} \psi(x) - \omega^\lambda{}_\nu x^\nu \partial_\lambda \psi(x) \\ &= -i \frac{1}{2} \omega_{\mu\nu} \left[S^{\mu\nu} + \hat{L}^{\mu\nu} \right] \psi(x) = -i \frac{1}{2} \omega_{\mu\nu} \hat{J}^{\mu\nu} \psi(x), \end{aligned} \tag{6.213}$$

the last line showing the separation into spin and orbital transformation.

Since the Dirac Lagrangian is Lorentz-invariant, it changes under Lorentz transformations like a scalar field:

$$\mathcal{L}'(x') = \mathcal{L}(x). \tag{6.214}$$

Infinitesimally, this amounts to

$$\delta_s \mathcal{L} = -(\partial_\mu \mathcal{L} x^\nu)\omega^\mu{}_\nu. \tag{6.215}$$

With the Lorentz transformations being symmetry transformation in the Noether sense, we calculate the *current of total four-dimensional angular momentum* extending the formulas (6.175) and (6.192) for scalar field and vector potential. It is again important to the hermitian Dirac Lagrangian density (3.447). The result is

$$J^{\mu\nu,\lambda} = \left(-i\frac{\partial\mathcal{L}}{\partial\partial_\lambda\psi}S^{\mu\nu}\psi - i\frac{\partial\mathcal{L}}{\partial\partial_\lambda\psi}\hat{L}^{\mu\nu}\psi + \mathrm{cc}\right) + \left[\delta^{\mu\lambda}\mathcal{L}x^\nu - (\mu\leftrightarrow\nu)\right]. \tag{6.216}$$

As before in (6.193) and (6.175), the orbital part of (6.216) can be expressed in terms of the canonical energy momentum tensor as

$$L^{\mu\nu,\lambda} = x^\mu\Theta^{\nu\lambda} - x^\nu\Theta^{\mu\lambda}. \tag{6.217}$$

The first term in (6.216) is the *spin current*

$$\Sigma^{\mu\nu,\lambda} = \frac{1}{2}\left(-i\frac{\partial\mathcal{L}}{\partial\partial_\lambda\psi}\sigma^{\mu\nu}\psi + \mathrm{cc}\right). \tag{6.218}$$

Inserting (6.152) and (3.472), this becomes explicitly

$$\Sigma^{\mu\nu,\lambda} = -\frac{i}{2}\bar{\psi}\gamma^\lambda\sigma^{\mu\nu}\psi = \frac{1}{2}\bar{\psi}\gamma^{[\mu}\gamma^\nu\gamma^{\lambda\}]}\psi = \frac{1}{2}\epsilon^{\mu\nu\lambda\kappa}\bar{\psi}\gamma^\kappa\psi. \tag{6.219}$$

The spin density is completely antisymmetric in the three indices.[5]

The conservation properties of the three currents are the same as in Eqs. (6.199)–(6.203).

Due to the presence of spin, the energy-momentum tensor is nonsymmetric.

6.10 Symmetric Energy Momentum Tensor

Since the presence of spin is the cause for the asymmetry of the canonical energy momentum tensor, it is suggestive that by an appropriate use of the spin current should be possible to construct a new modified momentum tensor

$$T^{\mu\nu} = \Theta^{\mu\nu} + \Delta\Theta^{\nu\mu} \tag{6.220}$$

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[5] This property is important for being able to construct a consistent quantum mechanics in a space with torsion. See H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics,*
World Scientific Publishing Co., Singapore 1995, Second extended edition, pp. 1–850.

which is symmetric, while still having the fundamental property of $\Theta^{\mu\nu}$, that the integral $P^\mu = \int d^3x T^{a0}$ is the total energy momentum vector of the system. This is be the case if $\Delta\Theta^{a0}$ is a three-divergence of a spatial vector. Such a construction was found by Belinfante in 1939. Belinfante introduced the tensor

$$T^{\mu\nu} = \Theta^{\mu\nu} - \frac{1}{2}\partial_\lambda(\Sigma^{\mu\nu,\lambda} - \Sigma^{\nu\lambda,\mu} + \Sigma^{\lambda\mu,\nu}) \tag{6.221}$$

whose symmetry is manifest, due to (6.201) and the symmetry of the last two terms under $\mu \leftrightarrow \nu$. Moreover, by the components

$$T^{a0} = \Theta^{a0} - \frac{1}{2}\partial_\lambda(\Sigma^{a0,c} - \Sigma^{0\lambda,\mu} + \Sigma^{\lambda\mu,0}) = x^\mu T^{\nu\lambda} - x^\nu T^{\mu\lambda} \tag{6.222}$$

which gives the same total angular momentum as the canonical expression (6.198):

$$J^{\mu\nu} = \int d^3x J^{\mu\nu,0}. \tag{6.223}$$

Indeed, the zeroth component of (6.222) is

$$x^\mu\Theta^{\nu 0} - x^\nu\Theta^{\mu 0} - \frac{1}{2}\left[\partial_k(\Sigma^{\mu 0,k} - \Sigma^{0k,\mu} + \Sigma^{k\mu,0})x^\nu - (\mu \leftrightarrow \nu)\right]. \tag{6.224}$$

Integrating the second term over d^3x and performing a partial integration gives, for $\mu = 0, \nu = i$

$$-\frac{1}{2}\int d^3x \left[x^0\partial_k(\Sigma^{i0,k} - \Sigma^{0k,i} + \Sigma^{ki,0}) - x^i\partial_k(\Sigma^{00,k} - \Sigma^{0k,0} + \Sigma^{k0,0})\right] = \int d^3x \Sigma^{0i,0}, \tag{6.225}$$

and for $\mu = i, \nu = j$

$$-\frac{1}{2}\int d^3x \left[x^i\partial_k(\Sigma^{j0,k} - \Sigma^{0k,j} + \Sigma^{kj,0}) - (i \leftrightarrow j)\right] = \int d^3x \Sigma^{ij,0}. \tag{6.226}$$

The right-hand sides are the contributions of the spin to the total angular momentum.

For the electromagnetic field, the spin current (6.196) reads, explicitly

$$\Sigma^{\mu\nu,\lambda} = -\frac{1}{c}\left[F^{\lambda\mu}A^\nu - (\mu \leftrightarrow \nu)\right]. \tag{6.227}$$

From this we calculate the Belinfante correction

$$\begin{aligned} \Delta\Theta^{\mu\nu} &= \frac{1}{2c}[\partial_\lambda(F^{\lambda\mu}A^\nu - F^{\lambda\nu}A^\mu) - \partial_\lambda(F^{\mu\nu}A^\lambda - F^{\mu\lambda}A^\nu) + \partial_\lambda(F^{\nu\lambda}A^\mu - F^{\nu\mu}A^\lambda)] \\ &= \frac{1}{c}\partial_\lambda(F^{\nu\lambda}A^\mu). \end{aligned} \tag{6.228}$$

Adding this to the canonical energy momentum tensor (6.143)

$$\Theta^{\mu\nu} = -\frac{1}{c}(F^\nu{}_\lambda\partial^\mu A^\lambda - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}), \tag{6.229}$$

we find the symmetric energy momentum tensor

$$T^{\mu\nu} = -\frac{1}{c}(F^{\nu}{}_{\lambda}F^{\mu\lambda} - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}) + \frac{1}{c}(\partial_{\lambda}F^{\nu\lambda})A^{\mu} \tag{6.230}$$

The last term vanishes due to the free Maxwell field equations, $\partial_{\lambda}F^{\mu\nu} = 0$ and can be dropped.

Note that the proof of the symmetry of $T^{\mu\nu}$ involves the field equations; via the divergence equation (6.201).

It is useful to see what happens to Belinfante's energy momentum tensor in the presence of an external current, i.e., if $T^{\mu\nu}$ is calculated from the Lagrangian

$$\mathcal{L} = -\frac{1}{4c}F_{\mu\nu}F^{\mu\nu} - \frac{1}{c^2}j^{\mu}A_{\mu}. \tag{6.231}$$

with an external current. The energy momentum tensor is

$$\Theta^{\mu\nu} = \frac{1}{c}\left(F^{\nu}{}_{\lambda}\partial^{\mu}A^{\lambda} - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}\right) + \frac{1}{c^2}g^{\mu\nu}j^{\lambda}A_{\lambda} \tag{6.232}$$

generalizing (6.24).

The spin current is the same as before, and we find Belinfante's energy momentum tensor

$$\begin{aligned} T^{\mu\nu} &= \Theta^{\mu\nu} + \frac{1}{c}\partial_{\lambda}(F^{\nu\lambda}A^{\mu}) &\quad (6.233)\\ &= -\frac{1}{c}(F^{\nu}{}_{\lambda}F^{\mu\lambda} - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}) + \frac{1}{c^2}g^{\mu\nu}j^{\lambda}A_{\lambda} + \frac{1}{c}(\partial_{\lambda}F^{\nu\lambda})A^{\mu}. \end{aligned}$$

Using Maxwell's equations $\partial_{\lambda}F^{\nu\lambda} = -j^{\lambda}$, the last term can also be rewritten as

$$-\frac{1}{c}j^{\nu}A^{\mu}. \tag{6.234}$$

This term prevents $T^{\mu\nu}$ from being symmetric, unless the current vanishes.

6.11 Internal Symmetries

In quantum field theory, an important role by classifying various actions is played by *internal symmetries*. They do not involve any change in the spacetime coordinate of the fields, i.e., they have the form

$$\phi'(x) = e^{-i\alpha G}\phi(x) \tag{6.235}$$

where G are the generators of some Lie group and α the associated transformation parameters. The field ϕ may have several indices on which the generator G acts as a matrix. The symmetry variation associated with (6.235) is obviously

$$\delta_s\phi'(x) = -i\alpha G\phi(x) \tag{6.236}$$

The most important example is that of a complex field ϕ and a generator $G = 1$, where (6.235) is simply a multiplication by a constant phase factor. One also speaks of U(1)-symmetry. Other important examples are those of a triplet or an octet of fields ϕ_i with G being the generators of an SU(2) vector representation or an SU(3) octet representation [the adjoint representations of these groups defined for Lie algebras in Eq. (3.79)]. The first case is associated with charge conservation in electromagnetic interactions, the other two with isospin and SU(3) invariance in strong interactions. The latter symmetries are, however, not exact.

6.11.1 U(1)-Symmetry and Charge Conservation

Given a Lagrangian density $\mathcal{L}(x) = \mathcal{L}(\phi(x), \partial\phi(x), x)$ depending only on the absolute squares $|\phi|^2, |\partial\phi|^2, |\phi\partial\phi|$. Then $\mathcal{L}(x)$ is invariant under U(1)-transformations

$$\delta_s\phi(x) = -i\phi(x) \tag{6.237}$$

i.e., $\delta_s L = 0$. By the chain rule of differentiation we find, using the Euler-Lagrange equation

$$\delta_s\mathcal{L} = \left(\frac{\partial\mathcal{L}}{\partial\phi} - \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial_\mu\phi}\right)\delta_s\phi + \left[\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\delta_s\phi\right] = 0 \tag{6.238}$$

Inserting (6.237), we find that

$$j_\mu = -\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\phi \tag{6.239}$$

is a conserved current.

For a free relativistic complex scalar field with a Lagrangian density

$$\mathcal{L}(x) = \partial_\mu\varphi^*\partial_\mu\varphi - m^2\varphi^*\varphi \tag{6.240}$$

we have to add the contributions of real and imaginary parts of the field ϕ in formula (6.239), and obtain the conserved current

$$j_\mu = -i\varphi^* \overleftrightarrow{\partial_\mu} \varphi \tag{6.241}$$

where $\varphi^* \overleftrightarrow{\partial_\mu} \varphi$ denotes the left-minus-right derivative:

$$\varphi^* \overleftrightarrow{\partial} \varphi \equiv \varphi^*\partial_\mu\varphi - (\partial_\mu\varphi^*)\varphi. \tag{6.242}$$

For a free Dirac field, we find from (6.239) the conserved current

$$j^\mu(x) = \bar\psi(x)\gamma^\mu\psi(x). \tag{6.243}$$

6.11.2 SU(N)-Symmetry

For more general internal symmetry groups, the symmetry variations have the form

$$\delta_s\varphi = -i\alpha_i G_i\varphi, \tag{6.244}$$

and the conserved currents are

$$j_i^\mu = -i\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}G_i\varphi \tag{6.245}$$

6.11.3 Broken Internal Symmetries

The physically important symmetries SU(2) of isospin and SU(3) are not exact. The Lagrange density is not strictly zero. In this case we remember the alternative derivation of the conservation law from (6.112). We introduce the spacetime-dependent parameters $\alpha(x)$ and conclude from the extremality property of the action that

$$\partial_\mu\frac{\partial\mathcal{L}^\epsilon}{\partial\partial_\mu\alpha_i(x)} = \frac{\partial\mathcal{L}^\epsilon}{\partial\alpha_i(x)} \tag{6.246}$$

This implies the divergence law for the above derived current

$$\partial_\mu j_i^\mu(x) = \frac{\partial\mathcal{L}^\epsilon}{\partial\alpha_i}. \tag{6.247}$$

6.12 Generating the Symmetry Transformations on Quantum Fields

As in quantum mechanical systems, the charges associated with the conserved currents obtained in the previous section can be used to generate the transformations of the fields from which they were derived. One merely has to invoke the canonical field commutation rules.

As an important example, consider the currents (6.245) of an internal U(N)-symmetry. Their charges

$$Q^i = -i\int d^3x\frac{\partial\mathcal{L}}{\partial\partial_\mu\varphi}G_i\varphi \tag{6.248}$$

can be written as

$$Q^i = -i\int d^3x\pi G_i\varphi, \tag{6.249}$$

where $\pi(x) \equiv \partial\mathcal{L}(x)/\partial\partial_\mu\varphi(x)$ is the canonical momentum of the field $\varphi(x)$. After quantization, these fields satisfy the canonical commutation rules:

$$\begin{aligned} [\pi(\mathbf{x},t),\varphi(\mathbf{x}',t)] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}'),\\ [\varphi(\mathbf{x},t),\varphi(\mathbf{x}',t)] &= 0,\\ [\pi(\mathbf{x},t),\pi(\mathbf{x}',t)] &= 0. \end{aligned} \tag{6.250}$$

From this we derive directly the commutation rule between the quantized charges (6.249) and the field $\varphi(x)$:

$$[Q^i, \hat{\varphi}(x)] = -\alpha^i G_i \varphi(x) \tag{6.251}$$

We also find that the commutation rules among the quantized charges

$$[\hat{Q}^i, \hat{Q}^j] = [G^i, G^j]. \tag{6.252}$$

Since these coincide with those of the matrices G_i this proves that the operators Q^i form a representation of the generators of symmetry group in the Fock space.

It is important to realize that the commutation relations (6.251) and (6.252) remain valid also in the presence of symmetry braking terms as long as these do not contribute to the canonical momentum of the theory. Such terms are called *soft symmetry braking terms*. The charges are no longer conserved, so that we must attach a time argument to the commutation relations (6.251) and (6.252). All times in these relations must be the same, in order to invoke the euqal-time canonical commutation rules.

The most important example is the commutation relation (6.91) which holds also in the presence of a potential $V(q)$ in the Hamiltonian. This breakes translational symmetry, but does not contribute to the canonical momentum $p = \partial L/\partial \dot{q}$. In this case, the relation generalizes to

$$\epsilon^j = i\epsilon^i [\hat{p}^i(t), \hat{x}^j(t)], \tag{6.253}$$

which is correct thanks to the validity of the canonical commutation relations (6.89) at arbitrary equal times, also in the presence of a potential.

Another important example are the commutation rules of the conserved charges associated with the Lorentz generators (6.217):

$$J^{\mu\nu} \equiv \int d^3x J^{\mu\nu,0}(x), \tag{6.254}$$

which are the same as those of the 4 × 4-matrices (3.82) and those of the quantum mechanical generators (6.95):

$$[\hat{J}^{\mu\nu}, \hat{J}^{\mu\lambda}] = -ig^{\mu\mu} \hat{J}^{\nu\lambda}. \tag{6.255}$$

The generators $J^{\mu\nu} \equiv \int d^3x J^{\mu\nu,0}(x)$, are sums $J^{\mu\nu} = L^{\mu\nu}(t) + \Sigma^{\mu\nu}(t)$ of charges (6.202) associated with orbital and spin rotations. According to (6.203), these individual charges are time dependent, only their sum being conserved. Nevertheless, they both generate Lorentz transformations: $L^{\mu\nu}(t)$ on the spacetime argument of the fields, and $\Sigma^{\mu\nu}(t)$ on the spin indices. As a consequence, they both satisfy the commutation relations (6.255):

$$\begin{aligned} [\hat{L}^{\mu\nu}, \hat{L}^{\mu\lambda}] &= -ig^{\mu\mu} \hat{L}^{\nu\lambda}, \\ [\hat{\Sigma}^{\mu\nu}, \hat{\Sigma}^{\mu\lambda}] &= -ig^{\mu\mu} \hat{\Sigma}^{\nu\lambda}. \end{aligned} \tag{6.256}$$

The commutators (6.252) have played an important role in developing a theory of strong interactions, where they first appeared in the form of a *charge algebra* of the broken symmetry SU(3) × SU(3) of weak and electromagnetic charges. This symmetry will be discussed in more detail in Chapter 10.

6.13 Energy Momentum Tensor of a Relativistic Massive Point Particle

If we want to study energy and momentum of charged relativistic point particles in an electromagnetic field it is useful to consider the action (6.65) with (6.69) as an integral over a Lagrangian density:

$$\mathcal{A}=\int d^4x\mathcal{L}(x), \qquad \text{with} \quad \mathcal{L}(x)=\int_{\tau_a}^{\tau_b} L(x'^{\mu}(\tau))\delta^{(4)}(x-x(\tau)). \tag{6.257}$$

Then we can derive for point particles similar local conservation laws as for fields. Instead of doing this, however, we shall simply take the already known global conservation laws and convert them into the local ones by inserting appropriate δ-functions with the help of the trivial identity

$$\int d^4x\delta^{(4)}(x-x(\tau))=1. \tag{6.258}$$

Consider for example the conservation law (6.71) for the momentum (6.72). With the help of (6.258) this becomes

$$0=-\int d^4x\int_{-\infty}^{\infty} d\tau\left[\frac{d}{d\tau}p_\lambda(\tau)\right]\delta^{(4)}(x-x(\tau)). \tag{6.259}$$

Note that in this expression the boundaries of the four volume contain the information on initial and final times. We then perform a partial integration in τ, and rewrite (6.259) as

$$\begin{aligned} 0 \;=\; & -\int d^4x\int_{-\infty}^{\infty} d\tau\frac{d}{d\tau}\left[p_\lambda(\tau)\delta^{(4)}(x-x(\tau))\right] \\ & +\int d^4x\int_{-\infty}^{\infty} d\tau p_\lambda(\tau)\partial_\tau\delta^{(4)}(x-x(\tau)). \end{aligned} \tag{6.260}$$

The first term vanishes if the orbits come from and disappear into infinity. The second term can be rewritten as

$$0=-\int d^4x\partial_\nu\left[\int_{-\infty}^{\infty} d\tau p_\lambda(\tau)\frac{dx^\nu}{d\tau}\delta^{(4)}(x-x(\tau))\right]. \tag{6.261}$$

This shows that

$$\Theta^{\lambda\nu}(x)\equiv\int_{-\infty}^{\infty} d\tau p^\lambda(\tau)\frac{dx^\nu}{d\tau}\delta^{(4)}(x-x(\tau)) \tag{6.262}$$

is conserved:

$$\partial_\nu\Theta^{\lambda\nu}(x)=0. \tag{6.263}$$

This is the energy momentum tensor of a massive point particle.

The total momenta are obtained from the spatial integrals over $\Theta^{\lambda 0}$:

$$P^{\mu}(t) \equiv \int d^3x \Theta^{\lambda 0}(x) = p^{\mu}(t). \tag{6.264}$$

For point particles, they coincide with the canonical momenta. If the Lagrangian depends only on x'^{μ}, these are constants of motion.

The Lorentz invariant quantity

$$M^2 = P^2 = g_{\mu\nu} P^{\mu} P^{\nu} \tag{6.265}$$

is called the *total mass* of the system.

Subjecting the orbits $x^{\mu}(\tau)$ to

Lorentz transformations according to the rules of the last section we find the currents of total angular momentum

$$L^{\mu\nu,\lambda} \equiv x^{\mu}\Theta^{\nu\lambda} - x^{\nu}\Theta^{\mu\lambda}, \tag{6.266}$$

to satisfy the conservation law:

$$\partial_{\lambda} L^{\mu\nu,\lambda} = 0. \tag{6.267}$$

A spatial integral over the zeroth component of the current $L^{\mu\nu,\lambda}$ yields the conserved charges:

$$L^{\mu\nu}(t) \equiv \int d^3x L^{\mu\nu,\lambda 0}(x) = x^{\mu} p^{\nu}(t) - x^{\nu} p^{\mu}(t). \tag{6.268}$$

6.14 Energy Momentum Tensor of Charged Particles in an Electromagnetic Field

Let us also consider an important combination of a charged point particle and an electromagnetic field Lagrangian

$$\mathcal{A} = -mc \int_{\tau_{\mu}}^{\tau_{\nu}} d\tau \sqrt{g_{\mu\nu} x'^{\mu} x'^{\nu}} - \frac{1}{4c} \int d^4x F_{\mu\nu} F^{\mu\nu} - \frac{e}{c^2} \int_{\tau_{\mu}}^{\tau_{\nu}} d\tau \frac{dx^{\mu}(\tau)}{d\tau} A_{\mu}(x(\tau)). \tag{6.269}$$

By varying the action in the particle orbits, we obtain the Lorentz equation of motion

$$\frac{dp^{\mu}}{d\tau} = (\frac{e}{c}) F^{\mu}{}_{\nu} \frac{dx^{\nu}}{d\tau}. \tag{6.270}$$

By varying the action in the vector potential, we find the Maxwell-Lorentz equation

$$-\partial_{\nu} F^{\mu\nu} = \frac{e}{c} \frac{dx^{\nu}}{d\tau}. \tag{6.271}$$

The action (6.269) is invariant under translations of the particle orbits and the electromagnetic fields. The first term is obviously invariant, since it depends only on the derivatives of the orbital variables $x^\mu(\tau)$. The second term changes under translations by a pure divergence [recall (6.124)]. Also the interaction term is invariant, ehich is seen as follows: Since the symmetry variation changes

$$A_\mu(x^\nu) \to A'_\mu(x^\nu) = A_\mu(x^\nu + \epsilon^\nu) \tag{6.272}$$

and $x^\nu(\tau) \to x^\nu(\tau) - \epsilon^\nu$, we have

$$\begin{array}{rcl} A_\mu(x(\tau)) & \to & A_\mu(x(\tau)) \\ \dfrac{dx^\mu}{d\tau} & \to & \dfrac{dx^\mu}{d\tau}. \end{array} \tag{6.273}$$

Hence altogether

$$\delta_{\rm s}\mathcal{A} = \epsilon^\nu \partial_\nu \mathcal{L}^{\rm em}. \tag{6.274}$$

We now we calculate the same variation once more invoking the equations of motion. This gives

$$\delta_{\rm s}\mathcal{A} = \int d\tau \frac{d}{d\tau}\frac{\partial L^{\rm m}}{\partial x'^\mu}\delta_{\rm s} x^\mu + \int d^4x \frac{\partial \mathcal{L}^{\rm em}}{\partial \partial_\lambda A^\mu}\delta_{\rm s} A^\mu. \tag{6.275}$$

The first term can be treated as in (6.71) - (6.261) after which it acquires the form

$$\begin{aligned} -\int_{\tau_\mu}^{\tau_\nu} d\tau \frac{d}{d\tau}(p_\mu + \frac{e}{c}A_\mu) \qquad\qquad\qquad\qquad\qquad\qquad & \qquad (6.276) \\ = -\int d^4x \int_{-\infty}^{\infty} d\tau \frac{d}{d\tau}\left[\left(p_\mu + \frac{e}{c}A_\mu\right)\delta^{(4)}(x - x(\tau)\right] & \\ +\int d^4x \int_{-\infty}^{\infty} d\tau \left(p_\mu + \frac{e}{c}A_\mu\right)\frac{d}{d\tau}\delta^{(4)}(x - x(\tau)) & \end{aligned}$$

and thus, after dropping boundary terms,

$$= \partial_\lambda \int d^4x \int_{-\infty}^{\infty} d\tau \left(p_\mu + \frac{e}{c}A_\mu\right)\frac{dx^\lambda}{d\tau}\delta^{(4)}(x - x(\tau)). \tag{6.277}$$

The electromagnetic part is the same as before, since the interaction contains no derivative of the gauge field. In this way we find the canonical energy momentum tensor

$$\begin{aligned} \Theta^{\mu\nu}(x) &= \int d\tau \left(p^\mu + \frac{e}{c}A^\mu\right)\frac{dx^\nu}{d\tau}\delta^{(4)}(x - x(\tau)) \\ &\quad -\frac{1}{c}\left(F^\nu{}_\lambda \partial^\mu A^\lambda - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}\right). \end{aligned} \tag{6.278}$$

Let us check its conservation by calculating the divergence:

$$\begin{aligned} \partial_\nu \Theta^{\mu\nu}(x) &= \int d\tau \left(p + \frac{e}{c}A_\mu\right)\frac{dx^\nu}{d\tau}\partial_\nu \delta^{(4)}(x - x(\tau)) \\ &\quad -\frac{1}{c}\partial_\nu F^\nu{}_\lambda \partial^\mu A^\lambda - \frac{1}{c}\left[F^\nu{}_\lambda \partial_\nu \partial^\mu A^\lambda - \frac{1}{4}\partial^\mu(F^{\lambda\kappa}F_{\lambda\kappa})\right]. \end{aligned} \tag{6.279}$$

The first term is, up to a boundary term, equal to

$$\begin{aligned} & -\int d\tau \left(p^\mu + \frac{e}{\tau}A^\mu\right) \frac{d}{d\tau}\delta^{(4)}(x - x(\tau)) \\ & = \int d\tau \left[\frac{d}{d\tau}\left(p^\mu + \frac{e}{c}A^\mu\right)\right] \delta^{(4)}(x - x(\tau)). \end{aligned} \tag{6.280}$$

Using the Lorentz equation of motion (6.270), this becomes

$$\frac{e}{c}\int_{-\infty}^{\infty} d\tau \left(F^\mu{}_\nu \frac{dx^\nu}{d\tau} + \frac{d}{d\tau}A^\mu\right) \delta^{(4)}(x - x(\tau)). \tag{6.281}$$

Inserting the Maxwell equation $\partial_\nu F^{\mu\nu} = -e \int d\tau (dx^\mu/d\tau)\delta^{(4)}(x - x(\tau))$, the second term in Eq. (6.279) can be rewritten as

$$-\frac{e}{c}\int_{-\infty}^{\infty} d\tau \frac{dx_\lambda}{d\tau}\partial^\mu A^\lambda \delta^{(4)}(x - x(\tau)), \tag{6.282}$$

which is the same as

$$-\frac{e}{c}\int d\tau \left(\frac{dx_\mu}{d\tau}F^{\mu\lambda} + \frac{dx_\lambda}{d\tau}\partial^\lambda A^\mu\right) \delta^{(4)}(x - x(\tau)), \tag{6.283}$$

thus canceling (6.281). The third term in (6.279), finally is equal to

$$-\frac{1}{c}\left[F^\nu{}_\lambda \partial^\mu F_\nu{}^\lambda - \frac{1}{4}\partial^\mu (F^{\lambda\kappa}F_{\lambda\kappa})\right] \tag{6.284}$$

due to the antisymmetry of $F^{\nu\lambda}$. With the help of the homogeneous Maxwell equation, the Bianchi identity

$$\partial_\lambda F_{\mu\nu} + \partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} = 0,$$

we see that this term vanishes identically.

It is easy to construct from (6.278) Belinfante's symmetric energy momentum tensor. We merely observe that the spin density is entirely due to the vector potential, and hence the same as before [see (6.227)]

$$\Sigma^{\mu\nu,\lambda} = -\frac{1}{c}\left[F^{\lambda\mu}A^\nu - (\mu \leftrightarrow \nu)\right]. \tag{6.285}$$

Hence the additional piece to be added to the canonical energy momentum tensor is again [see (6.228)]

$$\begin{aligned} \Delta\Theta^{\mu\nu} &= \frac{1}{c}\partial_\lambda (F^{\mu\nu}A^\mu) \\ &= \frac{1}{2}(\partial_\lambda F^{\nu\lambda}A^\mu + F^{\nu\lambda}\partial_\lambda A^\mu). \end{aligned} \tag{6.286}$$

The second term in this expression serves to symmetrize the electromagnetic part of the canonical energy-momentum tensor and brings it to the Belinfante form:

$$\overset{\rm em}{T}{}^{\mu\nu} = -\frac{1}{c}\left(F^{\nu}{}_{\lambda}F^{\mu\lambda} - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}\right). \qquad (6.287)$$

The first term in (6.286), which in the absence of charges vanished, is now just what is needed to symmetrize the matter part of $\Theta^{\mu\nu}$. Indeed, using once more Maxwell's equation, it becomes

$$-\frac{e}{c}\int d\tau \frac{dx^{\nu}}{d\tau}A^{\mu}\delta^{(4)}(x - x(\tau)) \qquad (6.288)$$

thus canceling the corresponding term in (6.278). In this way we find that the total energy momentum tensor of charged particles plus electromagnetic fields is simply the term of the two symmetric energy momentum tensor.

$$\begin{aligned} T^{\mu\nu} &= \overset{\rm m}{T}{}^{\mu\nu} + \overset{\rm em}{T}{}^{\mu\nu} && (6.289)\\ &= \frac{1}{m}\int_{-\infty}^{\infty} d\tau u^{\mu}u^{\nu}\delta^{(4)}(x - x(\tau)) - \frac{1}{c}\left(F^{\nu}{}_{\lambda}F^{\mu\lambda} - \frac{1}{4}g^{\mu\nu}F^{\lambda\kappa}F_{\lambda\kappa}\right) \end{aligned}$$

For completeness, let us cross check also its conservation. Forming the divergence $\partial_{\nu}T^{\mu\nu}$, the first term gives now only

$$\frac{e}{c}\int d\tau F^{\mu}{}_{\nu}\frac{dx^{\nu}}{d\tau} \qquad (6.290)$$

in contrast to (6.281), which is canceled by the divergence in the second term

$$-\frac{1}{c}\partial_{\nu}F^{\nu}{}_{\lambda}F^{\mu\lambda} = -\frac{e}{c}\int d\tau \frac{dx_{\lambda}}{d\tau}F^{\mu\lambda}, \qquad (6.291)$$

in contrast to (6.283).

Notes and References

For more details on the canonical formalism see

S. Schweber, *Relativistic Quantum Fields*, Harper and Row, N.Y., N.Y., 1961
A.O. Barut, *Electrodynamics and Classical Theory of Fields and Particles*, MacMillan, New York, N.Y. 1964
J.D. Jackson, *Classical Electrodynamics*, John Wiley + Sons, New York, N.Y., 1975
L. Landau, E. Lifshitz, *The Classical Theory of Fields*, Addison-Wesley, Reading, Mess., 1951

The Belinfante energy momentum tensor is discussed further in

H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. II *Stresses and Defects*, World Scientific Publishing Co., Singapore 1989, pp. 744-1443.

7

Scattering and Decay of Particles

So far we have discussed only free particles. If we want to detect the presence and detailed properties of any of them it is necessary to perform scattering experiments or to observe their decay products. In this chapter, we shall develop an appropriate quantum mechanical description of such processes.

7.1 INTERACTION PICTURE

Consider a quantum mechanical system whose Schrödinger equation

$$\hat{H}|\psi_S(t)\rangle = i\partial_t|\psi_S(t)\rangle \tag{7.1}$$

cannot be solved analytically (here we use natural units with $\hbar$=1). The standard methods of gaining information on such a system come from perturbation theory. The Hamilton operator is separated into a time-independent part $\hat{H}_0$ whose Schrödinger equation

$$\hat{H}_0|\psi_S(t)\rangle = i\partial_t|\psi_S(t)\rangle \tag{7.2}$$

is solvable, and a remainder $\hat{V}$ called interaction. The total Hamilton operator is

$$\hat{H} = \hat{H}_0 + \hat{V}. \tag{7.3}$$

The operator $\hat{H}_0$ is called the *unperturbed Hamiltonian*, the interaction $\hat{V}$ is often called the *perturbation*. For the sake of a simple notation we have omitted the hats on top of all operators without danger of confusion. The time-dependent state $|\psi_S(t)\rangle$ carries a subscript S to indicate the fact that we are dealing with the Schrödinger picture. Observables are operators $\hat{O}_S\,(\mathbf{p},\mathbf{x},t)$ whose matrix elements between states yield transition amplitudes. The interaction will be assumed to be of finite range. This excludes, for the moment, the most important interaction potential, the Coulomb potential. As an example, we may assume the unperturbed Hamiltonian to describe a particle in a Rosen-Morse potential well

$$\langle\mathbf{x}|\hat{V}|\mathbf{x}\rangle = V(\mathbf{x}) = \frac{\text{const}}{\cosh^2|\mathbf{x}|}. \tag{7.4}$$

If the constant is sufficiently negative, the system has one or more discrete bound states. The important Coulomb potential does not fall directly into the class of potential considered. It must first be modified by multiplying it with a very small exponential screening factor. The consequences of the infinite range which arises when removing this factor will have to be discussed separately. The interaction $\hat{V}$ may in general depend explicitly on time.

The results will later be applied to quantum field theory. There, $\hat{H}_0$ will be a sum of the second-quantized Hamilton operator of all particles involved, and $\hat{V}$ some as yet unspecified short-range interaction between them. If the particles are all massive, all forces will be of short range. Moreover, the vacuum state is a discrete state which is well separated from all other states by an energy gap. The lowest excited state contains a single particle with the smallest mass at rest. This mass is the energy gap.

The other, equivalent, description of the system due to Heisenberg works with *time-independent* states which are equal to the Schrödinger states $|\psi_S(t)\rangle$ at a certain fixed time $t = t_0$, which we shall take to be $t_0 = 0$, for simplicity:

$$|\psi_H\rangle \equiv |\psi_S(0)\rangle = \hat{U}(t,0)^{-1}|\psi_S(t)\rangle. \tag{7.5}$$

When using time-independent states, the time dependence of the system is carried by *time-dependent* Heisenberg operators

$$\hat{O}_H(t) = \hat{U}(t,0)^{-1}\hat{O}_S\hat{U}(t,0). \tag{7.6}$$

Here $\hat{U}(t,0)$ is the unitary time evollution operator introduced in Section 1.4 which governs the motion of the Schrödinger state. It has the explicitly form [recall (1.205)]

$$\hat{U}(t,0) \;\; = \;\; \hat{T}\left(e^{-i\int_0^t dt'\,\hat{H}(t')}\right). \tag{7.7}$$

If $\hat{H}$ has no explicit time depencence, which we shall assume from now on, then $\hat{U}(t,0)$ has the explicit form $\hat{U}(t,0) = e^{i\hat{H}t/\hbar}$ and satisfies the *unitarity relations*

$$\hat{U}^{-1}(t,0) = \hat{U}^{\dagger}(t,0) = \hat{U}(0,t). \tag{7.8}$$

Then the relation (7.6) becomes

$$\hat{O}_H(t) = \hat{U}(t,0)^{-1}\hat{O}_S\hat{U}(t,0). \tag{7.9}$$

As far as perturbation theory is concerned it is useful to introduce yet a third description called the *Dirac* or *interaction picture.* Its states are related to the previous ones by

$$|\psi_I(t)\rangle = e^{i\hat{H}_0t}|\psi_S(t)\rangle = e^{i\hat{H}_0t}\hat{U}(t,0)|\psi_H\rangle. \tag{7.10}$$

They have the property that in the absence of interactions they become time independent and coincide, in this case, with the Heisenberg states (7.5). The interactions, however, drive $\psi_I(t)$ away from $\psi_H(t)$.

When using such states, the observables in the interaction picture are

$$\hat{O}_I(t) = e^{i\hat{H}_0 t}\hat{O}_S e^{-i\hat{H}_0 t} = e^{i\hat{H}_0 t} e^{-i\hat{H}t}\hat{O}_H e^{i\hat{H}t} e^{-i\hat{H}_0 t}. \tag{7.11}$$

These operators coincide, of course, with those of the Heisenberg picture in the absence of interactions. By definition, the unperturbed Schrödinger equation $\hat{H}_0|\psi(t)\rangle$ can be solved explicitly implying that the time dependence of the operators $\hat{O}_I(t)$

$$\frac{d}{dt}\hat{O}_I(t) = [\hat{H}_0, \hat{O}_I(t)] \tag{7.12}$$

is completely known. If the Schrödinger operator $\hat{O}_S$ is explicitly time dependent, this becomes

$$\frac{d}{dt}\hat{O}_I(t) = [\hat{H}_0, \hat{O}_I(t)] + [\dot{\hat{O}}_S(t)]_I, \tag{7.13}$$

where

$$[\dot{\hat{O}}_S(t)]_I \equiv e^{i\hat{H}_0 t}\dot{\hat{O}}_S(t) e^{-i\hat{H}_0 t}. \tag{7.14}$$

A state vector in the interaction picture moves according to the following equation of motion

$$\begin{aligned} i\partial_t|\psi_I(t)\rangle &= i\partial_t e^{i\hat{H}_0 t}|\psi_S(t)\rangle \\ &= -\hat{H}_0|\psi_I(t)\rangle + e^{i\hat{H}_0 t}\hat{H}e^{-i\hat{H}_0 t}|\psi_I(t)\rangle \\ &= \hat{V}_I(t)|\psi_I(t)\rangle \end{aligned} \tag{7.15}$$

where

$$\hat{V}_I(t) \equiv e^{i\hat{H}_0 t}\hat{V}_S e^{-i\hat{H}_0 t} \tag{7.16}$$

is the interaction picture of the potential $\hat{V}_S$. It is useful to introduce a unitary time evolution operator also for the interaction picture. It determines the evolution of the states by

$$|\psi_I(t)\rangle = \hat{U}_I(t, t_0)|\psi_I(t_0)\rangle. \tag{7.17}$$

Obviously, $\hat{U}_I(t, t_0)$ satisfies the same composition law as the previously introduced time translation operator $\hat{U}(t, t_0)$ in the Schrödinger picture:

$$\hat{U}_I(t, t_0) = \hat{U}_I(t, t')\hat{U}_I(t', t_0). \tag{7.18}$$

Using the differential equation (7.15) for the states we see that the operator $\hat{U}_I(t, t_0)$ satisfies

$$i\partial_t\hat{U}_I(t, t_0) = \hat{V}_I(t)\hat{U}_I(t, t_0). \tag{7.19}$$

This equation can be integrated resulting in the Neumann-Liouville expansion [recall (1.200), (1.201)]

$$\begin{aligned}\hat{U}_I(t,t_0) &= 1 - i\int_{t_0}^{t} dt_1 \hat{V}_I(t_1) + \frac{(-i)^2}{2!}\hat{T}\int_{t_0}^{t} dt_1 dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2) + \dots \\ &\equiv \hat{T}\exp\left[-i\int_{t_0}^{t} dt'\,\hat{V}_I(t')\right]. \end{aligned} \tag{7.20}$$

The expansion holds for $t > t_0$ and respects the initial condition $\hat{U}_I(t_0, t_0) = 1$.

Note that the differential equation (7.19) for $\hat{U}_I(t,t_0)$ implies that $\hat{U}_I(t,t_0)$ satisfies an integral equation

$$\hat{U}_I(t,t_0) = 1 - i\int_{t_0}^{t} dt' \hat{V}_I(t')\hat{U}_I(t',t_0). \tag{7.21}$$

Indeed, iterating this we recover the Neumann-Liouville expansion (7.20).

For $t < t_0$, we may use the relation (7.8) according to which $\hat{U}(t,t_0) = \hat{U}^{-1}(t_0,t)$ and the expansion is again applicable. The time-ordering operator T makes sure that the operators $\hat{V}_I(t_i)$ in the expansion appear in chronological order with all later $\hat{V}_I(t_i)$ standing to the left of earlier ones.

If $\hat{V}$ and therefore $\hat{H}$ has no explicit time dependence, the Schrödinger state evolves via the simple exponential time evolution operator

$$|\psi_S(t)\rangle = \hat{U}(t,t_0)|\psi_S(t_0)\rangle = e^{-i\hat{H}(t-t_0)}|\psi_S(t_0)\rangle. \tag{7.22}$$

Combining this with (7.10) we see that

$$\hat{U}_I(t,t_0) = e^{i\hat{H}_0 t} e^{-i\hat{H}(t-t_0)} e^{-i\hat{H}_0 t_0}. \tag{7.23}$$

If the potential $\hat{V}$ depends explicitly on time, this has to be replaced by [recall (7.7)]

$$\begin{aligned}\hat{U}_I(t,t_0) &= e^{i\hat{H}_0 t}\hat{T}\left(e^{-i\int_{t_0}^{t} dt'\,\hat{H}(t')}\right)e^{-i\hat{H}_0 t_0} \\ &= e^{i\hat{H}_0 t}\hat{U}(t,t_0)e^{-i\hat{H}_0 t_0}. \end{aligned} \tag{7.24}$$

For a time-independent $\hat{H}$, this relation shows that $\hat{U}_I(t,t_0)$ satisfies the same unitarity relations (7.8) as $\hat{U}(t,t_0)$:

$$\hat{U}_I^{-1}(t,0) = \hat{U}_I^{\dagger}(t,0) = \hat{U}_I(0,t). \tag{7.25}$$

Note that the Heisenberg representation (7.6) of an arbitrary operator is obtained from the interaction representation (7.11) via

$$\begin{aligned}\hat{O}_{\hat{H}}(t) &= \hat{U}^{-1}(t,0)e^{-i\hat{H}_0 t}\hat{O}_I(t)e^{i\hat{H}_0 t}\hat{U}(t,0) \\ &= \hat{U}_I^{-1}(t,0)\hat{O}_I(t)\hat{U}_I(t,0) \end{aligned} \tag{7.26}$$

We have observed above that the operator in the interaction picture $\hat{O}_I(t)$ has a particularly simple time dependence. Its movement is determined by the unperturbed equation of motion (7.12). Thus, (7.26) establishes a relation between the complicated time dependence of the Heisenberg operator $\hat{O}_H(t)$ in the presence of interaction and the simple time dependence of $\hat{O}_I(t)$ which reduces to the Heisenberg operator in the absence of an interaction.

Consider now a scattering process in which two initial particles approach each other from a large distance outside the range of their interactions. This implies that their states at a very early time $t \rightarrow -\infty$ obey the unperturbed Schrödinger theory, i.e., that their wave function $\psi_I(t)$ is time independent. The same thing will be true a very long time after the scattering has taken place. Let us study the behavior of the operator $\hat{U}_I(t, t_0)$ in the two limits of large positive and negative time arguments. In order to make all expressions well defined mathematically it is convenient to introduce a simple modification of the potential by multiplying it with a switching factor $e^{-\eta|t|}$:

$$\begin{aligned} \hat{V} &\rightarrow e^{-\eta|t|}\hat{V} \equiv \hat{V}^\eta(t), &(7.27)\\ \hat{V}_I(t) &\rightarrow e^{-\eta|t|}\hat{V}_I(t) \equiv \hat{V}_I^\eta(t) &(7.28)\end{aligned}$$

with an infinitesimal parameter η. As far as physical observations are concerned, such a factor must have little relevance since η can be chosen so that $\hat{V}$ remains unchanged over any finite interval of time. An immediate consequence of the prescription (7.27), however, is that for $t \rightarrow \pm\infty$, the state vector in the interaction picture becomes time independent, due to (7.15): Let us denote the limiting states as $|\psi_{\substack{\text{in}\\ \text{out}}}\rangle$, i.e.,

$$|\psi_I(t)\rangle \underset{t\rightarrow\mp\infty}{\longrightarrow} |\psi_{\substack{\text{in}\\ \text{out}}}\rangle. \tag{7.29}$$

Using the time evolution operator, the limit (7.29) may be written as

$$\hat{U}_I(t,0)|\psi_I(0)\rangle \underset{t\rightarrow\mp\infty}{\longrightarrow} |\psi_{\substack{\text{in}\\ \text{out}}}\rangle \tag{7.30}$$

i.e., the operator $\hat{U}_I$ becomes a constant in the limit $t \rightarrow \mp\infty$. Inverting this relation we may write

$$|\psi_I(0)\rangle = \hat{U}_I(0,\mp\infty)|\psi_{\substack{\text{in}\\ \text{out}}}\rangle. \tag{7.31}$$

The operators

$$\hat{\Omega}^{(\pm)} \equiv \hat{U}_I(0,\mp\infty) \tag{7.32}$$

were first studied extensively by Møller[1] and are named after him. We shall now state their important properties which both are directly related to (7.31). We shall assume the common situation that $\hat{V}$ has no explicit time dependence except for the very slow switching factor (7.26). Suppose that $|\psi_{\substack{\text{in}\\\text{out}}}\rangle$ is a steady state solution of the time-independent unperturbed Schrödinger equation

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[1] C. Møller, Kgl. Danske Vidensk. Selsk. Mat.Fys. Medd *23*, No. 1, (1945).

$$\hat{H}_0|\psi_{\substack{\text{in}\\\text{out}}}\rangle = E|\psi_{\substack{\text{in}\\\text{out}}}\rangle. \tag{7.33}$$

Then $|\psi_I(0)\rangle$ solves the fully interacting Schrödinger equation with the same energy

$$\hat{H}|\psi_I(0)\rangle = E|\psi_I(0)\rangle. \tag{7.34}$$

The solution of this equation can immediately be found in the form of a perturbation series by inserting the Neumann-Liouville expansion (7.20) into Eq. (7.31):

$$\begin{aligned} |\psi_I(0)\rangle &= |\psi_{\text{in}}\rangle - i\int_{-\infty}^{0} dt'\hat{V}_I(t')|\psi_{\text{in}}\rangle \\ &\quad +(-i)^2\int_{-\infty}^{0} dt'\int_{-\infty}^{t} dt''\hat{V}_I(t')\hat{V}_I(t'')|\psi_{\text{in}}\rangle + \dots, \end{aligned} \tag{7.35}$$

With the help of (7.16) and inserting the damping factor as in Eq. (7.27) we see that the second term is equal to

$$-i\int_{-\infty}^{0} dt e^{\eta t} e^{i\hat{H}_0 t}\hat{V}e^{-i\hat{H}_0 t}|\psi_{\text{in}}\rangle. \tag{7.36}$$

By assumption, $|\psi_{\text{in}}\rangle$ is an eigenstate of $\hat{H}_0$ with energy E, and $\hat{V}$ is independent of time. Thus we can perform the integral and obtain

$$-i\int_{-\infty}^{0} dt e^{\eta t} e^{i(\hat{H}_0-E)t}\hat{V}|\psi_{\text{in}}\rangle = \frac{1}{E-\hat{H}_0+i\eta}\hat{V}|\psi_{\text{in}}\rangle. \tag{7.37}$$

Treating the other expansion terms in (7.35) likewise we arrive at the expansion

$$\begin{aligned} |\psi_I(0)\rangle &= |\psi_{\text{in}}\rangle + \frac{1}{E-\hat{H}_0+i\eta}\hat{V}|\psi_{\text{in}}\rangle \\ &\quad +\frac{1}{E-\hat{H}_0+i\eta}\hat{V}\frac{1}{E-\hat{H}_0+i\eta}\hat{V}|\psi_{\text{in}}\rangle + \dots \end{aligned} \tag{7.38}$$

In the second denominator we have replaced $2i\eta$ by $i\eta$ since η is infinitesimally small and it actual size is irrelevant. The infinite sum is recognized as an iterative solution of the equation

$$|\psi_I(0)\rangle = |\psi_{\text{in}}\rangle + \frac{1}{E-\hat{H}_0+i\eta}\hat{V}|\psi_I(0)\rangle, \tag{7.39}$$

which was found by Lippmann and Schwinger.[2] The fact that this is really a solution of Eq. (7.34) is easily verified by multiplying both sides with $E-\hat{H}_0$. In this equation we identify the Møller operator as

$$\hat{\Omega}^{(+)} = \hat{U}(0,-\infty) = 1 + \frac{1}{E-\hat{H}_0+i\eta}\hat{V}. \tag{7.40}$$

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[2] For a discussion see M. Gell-Mann and M. Goldberger, Phys. Rev. *91*, 398 (1953).

Because of this notation one often writes the scattering state $|\psi_I(0)\rangle$ in (7.39) as $|\psi^{(+)}\rangle$ and the equation itself as

$$|\psi^{(+)}\rangle = |\psi_{\rm in}\rangle + \frac{1}{E - \hat{H}_0 + i\eta}\hat{V}|\psi^{(+)}\rangle. \tag{7.41}$$

There also exists a Lippmann-Schwinger equation yielding a different set of interacting states $|\psi^{(-)}\rangle$ from the outgoing free state $|\psi_{\rm out}\rangle$:

$$|\psi^{(-)}\rangle = |\psi_{\rm in}\rangle + \frac{1}{E - \hat{H}_0 - i\eta}\hat{V}|\psi^{(-)}\rangle, \tag{7.42}$$

where the Møller operator is

$$\hat{\Omega}^{(-)} = \hat{U}(0, -\infty) = 1 + \frac{1}{E - \hat{H}_0 - i\eta}\hat{V}. \tag{7.43}$$

The only difference with respect to (7.40) is the sign of the $i\eta$-term.

In quantum-mechanical textbooks, this equation is usually discussed in the Schrödinger representation where the incoming state $\langle\mathbf{x}|\psi_{\rm in}\rangle$ is represented by a plane wave $\langle\mathbf{x}|\mathbf{k}\rangle = e^{i\mathbf{kx}}$ with $\hat{H}_0|\mathbf{k}\rangle = (\hbar\mathbf{k}^2/2M)|\mathbf{k}\rangle$ while

$$\langle\mathbf{x}|\frac{1}{E - \hat{H}_0 + i\eta}\hat{V}|\psi_I(0)\rangle$$

is an asymptotically spherical wave emerging from the scattering center. Then the equation reads, more explicitly,

$$\langle\mathbf{x}|\psi_I(0)\rangle = \langle\mathbf{x}|\mathbf{k}\rangle + \int\frac{d^3k}{(2\pi)^3}\langle\mathbf{x}|\mathbf{k}\rangle\frac{1}{E - \hbar^2\mathbf{k}^2/2M + i\eta}\int d^3x'\langle\mathbf{k}|\hat{V}|\mathbf{x}'\rangle\langle\mathbf{x}'|\psi_I(0)\rangle, \tag{7.44}$$

The amplitude for the scattering process is found as follows. Let $|a_{\rm in}\rangle$ be a complete set of incoming eigenstates of the unperturbed Schrödinger equation

$$\hat{H}_0|a_{\rm in}\rangle = E_a|a_{\rm in}\rangle \tag{7.45}$$

where a denotes the collection of all quantum numbers of these states. By applying the interaction operator $\hat{U}_I(t, -\infty)$, the states $|a_{\rm in}\rangle$, they are transformed into the time-dependent $|a_I(t)\rangle$. After a long time, these develop into time-independent states $|a_{\rm out}\rangle$. The energies E_a remain, of course, unchanged.

Let us analyze the outgoing states $|a_{\rm out}\rangle$

$$|a_{\rm out}\rangle = \hat{U}_I(\infty, -\infty)\,|a_{\rm in}\rangle \tag{7.46}$$

with respect to the incoming waves $|b_{\rm in}\rangle$. The scalar products $\langle b_{\rm in}|a_{\rm out}\rangle$ are obviously equal to the matrix elements of $\hat{U}_I(\infty, -\infty)$:

$$\langle b_{\rm in}|a_{\rm out}\rangle = \langle b_{\rm in}|\hat{U}_I(\infty, -\infty)\,|a_{\rm in}\rangle. \tag{7.47}$$

The right-hand side is defined as the *scattering matrix* or S-matrix:

$$S_{ba} = \langle b_{\rm in}|\hat{U}_I(\infty,-\infty)|a_{\rm in}\rangle. \tag{7.48}$$

The same name is also often used sloppily for the scattering operator

$$\hat{S} \equiv \hat{U}_I(\infty,-\infty) \tag{7.49}$$

itself. This can be written as a product of the two Møller operators (7.32):

$$S = \hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}. \tag{7.50}$$

Note that with $\hat{U}_I(t,t_0)$ being a unitary operator, the S-matrix is unitary and satisfies:

$$SS^\dagger = S^\dagger S = 1. \tag{7.51}$$

The Møller operators, however, are not unitary. As we shall see in the next section, the operators $\hat{\Omega}^{(\pm)\dagger}$ are inverse to $\hat{\Omega}^{(\pm)}$ only if $\hat{H}_0$ has no bound states and then only under multiplication from the left-had side:

$$\hat{\Omega}^{(\pm)\dagger}\hat{\Omega}^{(\pm)} = 1, \tag{7.52}$$

whereas from the right-hand side they yield a projection operator onto the subspace of continuous states of the Hamiltonian $\hat{H}$:

$$\hat{\Omega}^{(\pm)}\hat{\Omega}^{(\pm)\dagger} = \hat{P}_{\rm continuum}. \tag{7.53}$$

Only in an infinite-dimensional Hilbert space makes it possible that the left inverse is not equal to the right inverse.

7.2 DISCRETE STATES

The Møller operator has nontrivial properties with respect to the discrete spectrum of the unperturbed Hamiltonian $\hat{H}_0$ and the perturbed Hamiltonian $\hat{H}$. Let us first understand the difference between the quasi-unitarity relations (7.52) and (7.53). We denote by $|\varphi_a\rangle$ the continuum and by $|\varphi_\beta\rangle$ the bound states of $\hat{H}_0$, similarly by $|\psi_a^{(\pm)}\rangle$ the continuum and by $|\psi_\beta\rangle$ the bound states of $\hat{H}$ which solve the Lippmann-Schwinger equations (7.41) and (7.42), respectively, the latter being independent of which of the two Lippmann-Schwinger equations is used. These states satisfy the completeness relations

$$\sum_a|\varphi_a\rangle\langle\varphi_a| + \sum_\beta|\varphi_\beta\rangle\langle\varphi_\beta| = 1, \qquad \sum_a|\psi_a^{(\pm)}\rangle\langle\psi_a^{(\pm)}| + \sum_\beta|\psi_\beta\rangle\langle\psi_\beta| = 1, \tag{7.54}$$

Only the continuum states carry the distinctive label (±) since only these depend on the small quantity η in the Lippmann-Schwinger equation (7.41) and (7.42). The bound states are uniquely determined by the condition of quadratic integrability.

The Møller operators $\hat{\Omega}^{(\pm)}$ transform the continuum states $|\varphi_a\rangle$ into scattering states $|\psi^{(\pm)}\rangle$. Thus we can expand

$$\hat{\Omega}^{(\pm)} = \hat{U}(0, \mp\infty) = \sum_a |\psi_a^{(\pm)}\rangle\langle\varphi_a|, \qquad \hat{\Omega}^{(\pm)\dagger} = \hat{U}^\dagger(0, \mp\infty) = \sum_a |\varphi_a\rangle\langle\psi_a^{(\pm)}|. \tag{7.55}$$

From these expansions, we extract the following important properties of the Møller operators:

$$\hat{\Omega}^{(\pm)\dagger}|\psi_a^{(\pm)}\rangle = |\varphi_a\rangle, \qquad \hat{\Omega}^{(\pm)\dagger}|\psi_\beta\rangle = 0. \tag{7.56}$$

The second relation implies that

$$\hat{\Omega}^{(\pm)\dagger} P^0_{\text{bd}} = 0. \tag{7.57}$$

We further find

$$\hat{\Omega}^{(\pm)\dagger}\hat{\Omega}^{(\pm)} = \sum_{a,b} |\varphi_a\rangle\langle\psi_a^{(\pm)}|\psi_b^{(\pm)}\rangle\langle\varphi_a| = 1 - \sum_\beta |\varphi_\beta\rangle\langle\varphi_\beta| = 1 - P^0_{\text{bd}}, \tag{7.58}$$

the operator on the right-hand side it the projection on the bound states of $\hat{H}_0$. In the opposite order, the product yields

$$\hat{\Omega}^{(\pm)}\hat{\Omega}^{(\pm)\dagger} = \sum_{a,b} |\psi_a^{(\pm)}\rangle\langle\varphi_a|\varphi_b\rangle\langle\psi_b^{(\pm)}| = 1 - \sum_\beta |\psi_\beta\rangle\langle\psi_\beta| = 1 - \hat{P}_{\text{bd}}, \tag{7.59}$$

where $\hat{P}_{\text{bd}}$ projects onto the bound states of $\hat{H}$. The different orders of the products differ by the projection onto the bound states of $\hat{H}$.

For the S-matrix, on the other hand, this dependence on the order disappears and we find

$$\begin{aligned} S^\dagger S &= [\hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}]^\dagger[\hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}] = \hat{\Omega}^{(+)\dagger}\hat{\Omega}^{(-)}\hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)} = \hat{\Omega}^{(+)\dagger}\left(1-\hat{P}_{\text{bd}}\right)\hat{\Omega}^{(+)} \\ &= 1 - P^0_{\text{bd}}, \end{aligned} \tag{7.60}$$

and

$$SS^\dagger = \hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}\hat{\Omega}^{(+)\dagger}\hat{\Omega}^{(-)} = \hat{\Omega}^{(-)\dagger}\left(1 - \hat{P}_{\text{bd}}\right)\hat{\Omega}^{(-)} = \hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(-)} = 1 - P^0_{\text{bd}}. \tag{7.61}$$

The projection operator $\hat{P}_{\text{bd}}$ drops out because of (7.57).

By definition, the S-matrix is calculated only between states in the subspace of the Hilbert space formed by the continuous eigenstates of $\hat{H}_0$. In this subspace, the projection operator P^0_{bd} vanishes and we find $S^\dagger S = 1$ and $SS^\dagger = 1$, in either order, showing that the S-matrix is unitary.

An obvious properties of the Møller operator is

$$\hat{H}\hat{\Omega}^{(\pm)} = \hat{\Omega}^{(\pm)}\hat{H}_0, \qquad \hat{\Omega}^{(\pm)\dagger}\hat{H} = \hat{H}_0\hat{\Omega}^{(\pm)\dagger}, \tag{7.62}$$

from which we find immediately that S does not change the energy of the incoming continuum states since $[\hat{H}_0, S] = 0$:

$$\hat{H}_0 S = \hat{H}_0 \hat{\Omega}^{(-)\dagger} \hat{\Omega}^{(+)} = \hat{\Omega}^{(-)\dagger} \hat{H} \hat{\Omega}^{(+)} = \hat{\Omega}^{(-)\dagger} \hat{\Omega}^{(+)} \hat{H}_0 = S \hat{H}_0. \tag{7.63}$$

For scattering states which all lie in the continuum of $\hat{H}_0$, the size of η is irrelevant at all times as long as it is very small and has a fixed sign. In contrast, a discrete eigenstate of $\hat{H}_0$ has a singular η-dependence in the limit of small η. In order to understand this we observe that for any short-range potential, the two scattering particles lie practically all the time outside of each other's range. Only for a small time interval do they interact. The potential is not felt for large positive and negative times where the wave packets are separated by a large distance. The switching factor is therefore physically irrelevant for sufficiently small η. It cannot influence the physics of the system. For bound states, however, the particles interact with each other *all the time* with the same strength. In order to understand this consider a specific discrete state, assuming it to be well separated from the lower and higher states by a finite energy gap Δ. Then, for $\eta \ll \Delta$, the time dependence of $\hat{V}^\eta(t) = e^{-\eta|t|}\hat{V}$ is so slow that the interaction is, over a long time interval, incapable of causing transitions from the discrete state to a neighbor state. Such a slow time dependence is called *adiabatic*. For an adiabatically time-dependent potential $\hat{V}^\eta(t)$, the discrete state $|\psi(t)\rangle$ is at any time t_0 to a very good approximation the solution of the time-independent Schrödinger equation containing the time-independent potential $\hat{V}(t_0)$. The energy $E(t)$ of the discrete state $|\psi(t)\rangle$ is at any finite time equal to E. Only for very large times $|t| > \pm 1/\eta$ does the interaction become so weak that the state $|\psi(t)\rangle$ becomes an eigenstate of $\hat{H}_0$, and the energy $E(t)$ goes against the associated eigenvalue E_0 of the unperturbed Hamilton operator $\hat{H}_0$.

The Møller operators relate the wave functions $|\psi\rangle$ of the interacting system which satify the Schrödinger equation

$$(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle, \tag{7.64}$$

to the corresponding unperturbed wave function $|\psi_0\rangle$ satisfying

$$\hat{H}_0|\psi_0\rangle = E_0|\psi_0\rangle. \tag{7.65}$$

Formally, this correspondence can be defined uniquely by multiplying $\hat{V}$ by a coupling constant g and varying g from $g = 0$ where the system is free to $g = 1$, where it is fully interacting. The energy $E(g)$ and the associated discrete state $|\psi(g)\rangle$ are continuous functions of g interpolating between E_0 and E, and between $|\psi_0\rangle$ and $|\psi\rangle$, respectively.

The two Møller operators $\hat{\Omega}^{(\pm)}$ of Eq. (7.32) associated with the potential $\hat{V}_I^\eta$ carry a nondegenerate the discrete state $|\psi_0\rangle$ into two solutions of the interacting Schrödinger equation (7.64) as follows (*first Gell-Mann-Low formula*):[3]

$$|\psi^{(\pm)}\rangle = \lim_{\eta \to 0} \hat{U}_I^\eta\,(0, \mp\infty)\,|\psi_0\rangle \frac{1}{z_\eta^{(\pm)}}. \tag{7.66}$$

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[3] M. Gell-Mann and F. Low, Phys. Rev. *84*, 350 (1951).

To have a finite limit, the transformed state has been divided by a normalization factor $z_\eta^{(\pm)}$ defined by the expectation value

$$z_\eta^{(\pm)} \equiv \langle\psi_0|\hat{U}_I^\eta\,(0,\mp\infty)\,|\psi_0\rangle. \tag{7.67}$$

Let us denote the states on the right-hand side of (7.66) without the normalization factors by

$$|\eta^{(\pm)}\,\rangle \quad \equiv \hat{U}_I^\eta\,(0,\mp\infty)\,|\psi_0\rangle. \tag{7.68}$$

These states satisfy for small but fixed η the Schrödinger equation

$$\left[\hat{H}_0 + \hat{V}^\eta(0)\right]|\eta^{(\pm)}\,\rangle = E_\eta|\eta^{(\pm)} rangle, \tag{7.69}$$

where E_η is some η-dependent energy. The proof is based on the observation that in front of the state $|\psi_0\rangle$, the η-dependent Møller operators

$$\hat{\Omega}_\eta^{(\pm)} \equiv \hat{U}_I^\eta(0,\mp\infty) \tag{7.70}$$

satisfy the obvious commutation rule

$$\left[\hat{H}_0, \hat{U}_I^\eta\,(0,\mp\infty)\right]|\psi_0\rangle = \hat{H}_0|\eta^{(\pm)}\,\rangle - E_0|\eta^{(\pm)}\,\rangle. \tag{7.71}$$

We now expand $\hat{U}_I^\eta\,(0,\mp\infty)$ according to (7.20) as

$$\begin{aligned}\hat{U}_I^\eta\,(0,-\infty) &= \hat{T}\left(e^{-ig\int_{-\infty}^0 dt\,e^{\eta t}\hat{V}_I(t)}\right) \qquad (7.72)\\ &= \sum_{n=0}^\infty \frac{(-ig)^n}{n!}\int_{-\infty}^0 dt_1\cdots\int_{-\infty}^0 dt_n e^{\eta\sum_{i=1}^n t_i}\,\hat{T}\left(\hat{V}_I(t_1)\cdots\hat{V}_I(t_n)\right).\end{aligned}$$

The operators $\hat{V}_I(t)$ in the interaction picture have the time dependence (7.12) which yields

$$\frac{d}{dt}\hat{V}_I(t) = i\left[\hat{H}_0, \hat{V}_I(t)\right]. \tag{7.73}$$

Using (7.72) and (7.73) we find

$$\begin{aligned}\left[\hat{H}_0, \hat{U}_I^\eta\,(0,-\infty)\right] &= -i\sum_{n=0}^\infty \frac{(-ig)^n}{n!}\int_{-\infty}^0 dt_1\cdots\int_{-\infty}^0 dt_n e^{\eta\sum_{i=1}^n t_i}\\ &\qquad\times\sum_{i=1}^n\frac{\partial}{\partial t_i}\hat{T}\left(\hat{V}_I(t_i)\cdots\hat{V}_I(t_a)\right). \qquad (7.74)\end{aligned}$$

Since the integrand is symmetric in the time variables, we may replace the sum $\sum_{i=1}^n \partial/\partial t_i$ by n-times the time derivative $\partial/\partial t_n$. Taking the derivative $\partial/\partial t_n$ to the left of the switching factors $e^{\eta t_i}$, the integral becomes

$$\begin{aligned}&-i\sum_{n=0}^\infty\frac{(-ig)^n}{n!}n\int_{-\infty}^0 dt_1\cdots\int_{-\infty}^0 dt_{n-1}\int_{-\infty}^0 dt_n\times\frac{\partial}{\partial t_n}\left[e^{\eta\sum_{i=1}^n t_i}\hat{T}\left(\hat{V}_I(t_1)\cdots\hat{V}_I(t_n)\right)\right]\\ &+i\eta\sum_{n=0}^\infty\frac{(-ig)^n}{n!}n\int_{-\infty}^0 dt_1\cdots\int_{-\infty}^0 dt_n e^{\eta\sum_{i=1}^n t_i}\hat{T}\left(\hat{V}_I(t_1)\cdots\hat{V}^I(t_n)\right). \qquad (7.75)\end{aligned}$$

The second sum is equal to

$$i\eta g\frac{\partial}{\partial g}\hat{U}_I^\eta(0,-\infty)\,. \tag{7.76}$$

The first sum contains integrals over a pure derivatives which can be replaced by surface terms. Moreover, since the integrand vanishes at $t_n=-\infty$, only the $t_n=0$ -term contributes. The time $t_n=0$ is the latest of all time variables. Thus it can be moved to the left of the time-ordering symbol, and we arrive at the equation

$$\left[\hat{H}_0,\hat{U}_I^\eta(0,-\infty)\right]=-g\hat{V}_I(0)\hat{U}_I^\eta(0,-\infty)+i\eta g\frac{\partial}{\partial g}\hat{U}_I^\eta(0,-\infty)\,. \tag{7.77}$$

In a similar way we derive

$$\left[\hat{H}_0,\hat{U}_I^\eta(0,+\infty)\right]=-g\hat{V}_I(0)\hat{U}_I^\eta(0,+\infty)-i\eta g\frac{\partial}{\partial g}\hat{U}_I^\eta(0,+\infty)\,. \tag{7.78}$$

An important property of these formulas is that in the presence of a level shift, the second term on the right-hand side proportional to η is nonzero in the limit $\eta\to0$. To see this, take Eq. (7.77) and rewrite it in a slightly different way as

$$\begin{aligned}\hat{H}\hat{U}_I^\eta(0,\mp\infty) &= \left[\hat{H}_0+g\hat{V}_I(0)\right]\hat{U}_I^\eta(0,\mp\infty)\\ &= \hat{U}_I^\eta(0,\mp\infty)\,\hat{H}_0\pm i\eta g\frac{\partial}{\partial g}\hat{U}_I^\eta(0,\mp\infty)\,.\end{aligned} \tag{7.79}$$

If this equation is applied to the state $|\psi_0\rangle$, it shows that the state $|\eta^{(\pm)}$ *rangle* of (7.68) satisfies the modified Schrödinger equation

$$\hat{H}|\eta^{(\pm)}\rangle=\left(E_0\pm i\eta g\frac{\partial}{\partial g}\right)|\eta^{(\pm)}\rangle. \tag{7.80}$$

If we were to take the limit $\eta\to0$ carelessly, we would arrive at the equation $\hat{H}|\eta^{(\pm)}\rangle=E_0|\eta^{(\pm)}\rangle$ and arroneously conclude that $|\eta\rangle_\mp$ were solutions of the fully interacting Schrödinger equation with energy E_0. For the continuum states, this conclusion is indeed true and we have

$$\hat{H}\hat{U}_I(0,\mp\infty)=\hat{U}_I(0,\mp\infty)\,\hat{H}_0, \tag{7.81}$$

rather than (7.79), as stated before in Eq. (7.62). For the discrete states, the energy is in general shifted by the interaction. Hence the derivative $g(\partial/\partial g)|\eta^{(\pm)}\rangle$ must diverges like $1/\eta$ such as to give a finite contribution in (7.80). The origin of the divergence is a diverging normalization of the state $|\eta\rangle_\mp$. Thus is divergence is eliminated by forming the states on the right-hand side of (7.66):

$$|\psi_\eta^{(\pm)}\rangle\equiv|\eta^{(\pm)}\rangle\frac{1}{z_\eta^{(\pm)}}. \tag{7.82}$$

These have a definite limit for $\eta \to 0$. For these states, Eq. (7.80) implies

$$\hat{H}|\psi_\eta^{(\pm)}\rangle = \left(E_0 \pm i\eta g \frac{\partial}{\partial g} \log z_\eta^{(\pm)}\right) |\psi_\eta^{(\pm)}\rangle. \tag{7.83}$$

$$\Delta E = \lim_{\eta \to 0} i\eta g \frac{\partial}{\partial g} \log z_\eta^{(\pm)}. \tag{7.84}$$

The level shifts caused by the interaction are given by the formula

$$\Delta E = \lim_{\eta \to 0} i\eta g \frac{\partial}{\partial g} \log z_\eta^{(\pm)}. \tag{7.85}$$

The level shift can also be expressed in terms of the η-dependent S-matrix

$$\begin{aligned} S^\eta &= \hat{U}_I^\eta (\infty, -\infty) \\ &= \hat{U}_I^\eta (\infty, 0)\, \hat{U}_I^\eta (0, -\infty). \end{aligned} \tag{7.86}$$

Indeed, by multiplying Eq. (7.80) for $|\eta^{(+)}\rangle$ by $\langle\psi_\eta^{(+)}|$ from the left we find

$$\langle\psi_\eta^{(\pm)}|\hat{H} - E_0|\eta^{(\pm)}\rangle = \Delta E \langle\psi_\eta^{(\pm)}|\eta^{(\pm)}\rangle = \pm i\eta g \langle\psi_\eta^{(\pm)}|\partial_g|\eta^{(\pm)}\rangle, \tag{7.87}$$

such that with the abbreviation $\partial_g \equiv \partial/\partial g$:

$$\Delta E = \pm i\eta g \frac{\langle\psi_\eta^{(\pm)}|\partial_g|\eta^{(\pm)}\rangle}{\langle\psi_\eta^{(\pm)}|\eta^{(\pm)}\rangle} \tag{7.88}$$

$$= \pm i\eta g \frac{\langle\psi_0|\hat{U}_I^\eta (\pm\infty, 0)\, \partial_g \hat{U}_I^\eta (0, \mp\infty)\, |\psi_0\rangle}{\langle\psi_0|\hat{U}_I^\eta (\pm\infty, 0)\, \hat{U}_I^\eta (0, \mp\infty)\, |\psi_0\rangle}. \tag{7.89}$$

Similarly, taking the equation for $\langle\eta^{(\pm)}|$ and multiplying it by $|\psi_\eta^{(\pm)}\rangle$ from the right we find

$$\Delta E = \pm i\eta g \frac{\langle\psi_0| \left[\partial_g \hat{U}_I^\eta (\pm\infty, 0)\right] \hat{U}_I^\eta (0, \mp\infty)\, |\psi_0\rangle}{\langle\psi_0|\hat{U}_I^\eta (\pm\infty, 0)\, \hat{U}_I^\eta (0, \mp\infty)\, |\psi_0\rangle}. \tag{7.90}$$

Adding both results for the upper sign gives

$$\Delta E \;=\; i\frac{\eta}{2} g \frac{\partial}{\partial g} \log\langle\psi_0|S^\eta (\infty, -\infty)\, |\psi_0\rangle. \tag{7.91}$$

Note that the matrix element $\langle\psi_0|S^\eta (\infty, -\infty)$ is a pure phase $e^{i\varphi^\eta}$. This is seen as follows. The state $|\eta^{(+)}\rangle$ develop after an infinitely long time into $\hat{U}_I^\eta (\infty, -\infty)\, |\psi_0\rangle$. There it becomes again an eigenstate of $\hat{H}_0$ due to the commutation relation (7.63). Thus ist must coincide with $|\psi_0\rangle$ up to some overall factor $e^{i\varphi_\eta}$ (recall that $|\psi_0\rangle$ is nondegenerate by assumption). Hence we arrive at the level shift formula

$$\Delta E \;=\; = -\frac{\eta}{2} g \frac{\partial}{\partial g} \varphi^\eta. \tag{7.92}$$

One sometimes finds this result sated the opposite direction:

$$\varphi^\eta = -2\frac{1}{\eta}\int_0^g \frac{dg'}{g'}\Delta E(g'). \tag{7.93}$$

To lowest order in g, where $\Delta E \propto g$, the formula becomes

$$\varphi^\eta \approx -2\frac{g}{\eta}\Delta E + O\left(g^2\right). \tag{7.94}$$

This formula is sometimes used for a lowest-order calculations of the change of mass of a particle due to interactions.

Actually, in applications the exponential switching factor is somewhat difficult to handle. A much more direct way of cutting off the interaction consists in a step function along the time axis, i.e., by assuming the total interaction time to be finite. The connection between T and η is found from the correspondence between the integrals

$$\int_{-\infty}^{\infty} dt e^{-\eta|t|} = \frac{2}{\eta} \longrightarrow \int_{-T/2}^{T/2} dt = T. \tag{7.95}$$

Then we may write simpler

$$\varphi^\eta = -T\int_0^g \frac{dg'}{g'}\Delta E(g') \tag{7.96}$$

7.3 Scattering Amplitude

After this development it is straightforward to derive scattering amplitudes for a particle in an external potential $\hat{V}(\mathbf{x})$ of finite range. Imagine a scattering center with a region of nonzero potential concentrated around the origin. A wave packet of a given average momentum $\mathbf{p}$ and energy E approaches this region along the x-axis from negative infinity. As long as it is far from the scattering center it follows the free-particle Schrödinger equation

$$\hat{H}_0|\psi(t)\rangle = i\partial_t|\psi(t)\rangle, \tag{7.97}$$

with the unperturbed Hamiltonian $\hat{H}_0 = \mathbf{p}^2/2M$. As the particle approaches the potential, the state will be driven by the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. In the interaction representation we study the time evolution of a state which diagonalizes the unperturbed Hamiltonian $\hat{H}_0$ and see how it changes due to the interaction $\hat{V}_I \exp(-\eta|t|)$. The switching factor $\exp(-\eta|t|)$ enables us to remove the scattering potential long before the scattering happens. This frees us from the necessity of assuming the incoming wave to be localized in a packet long before the scattering process. Instead, we can take it to be a pure plane wave, a momentum eigenstate $|\mathbf{p}\rangle$, with an energy $E_\mathbf{p} = \mathbf{p}^2/2M$, solving the time-independent Schrödinger equation

$$\hat{H}_0|\mathbf{p}\rangle = E_\mathbf{p}|\mathbf{p}\rangle. \tag{7.98}$$

The incoming wave function $\langle \mathbf{x}|\mathbf{p}\rangle = e^{i\mathbf{p}\mathbf{x}/\hbar}$ has the same probability everywhere in space, also in the scattering region, but since $\hat{V}_I$ is switched off at large $|t|$, this will presents no problem in the description of the scattering process. The amplitude for the incoming state $|\mathbf{p}\rangle$ to be scattered into another eigenstate with momentum $|\mathbf{p}'\rangle$ is given by the matrix elements

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'|\hat{U}_I\,(\infty, -\infty)\,|\mathbf{p}\rangle. \tag{7.99}$$

Decomposing $\hat{U}_I\,(\infty, -\infty)$ into the product of Møller operators,

$$\hat{U}_I\,(\infty, -\infty) = \hat{U}_I\,(\infty, 0)\,\hat{U}_I\,(0, -\infty) = \hat{\Omega}^{(-)\dagger}\hat{\Omega}^{(+)}, \tag{7.100}$$

we can also write

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'^{(-)}|\mathbf{p}^{(+)}\rangle \tag{7.101}$$

where $|\mathbf{p}^{(\pm)}\rangle$ are the states

$$|\mathbf{p}^{(\pm)}\rangle \equiv \hat{\Omega}^{(\pm)}|\mathbf{p}\rangle. \tag{7.102}$$

The time evolution does not change the energy under the assumption of an infinitesimally small η, such that these states satisfy the full Schrödinger equation with the same energy $E = E_{\mathbf{p}}$:

$$\hat{H}|\mathbf{p}^{(\pm)}\rangle = E_{\mathbf{p}}|\mathbf{p}^{(\pm)}\rangle \tag{7.103}$$

It is useful to take advantage of this property of the scattering process by rewriting the matrix element (7.99) in another way using the explicit operator (7.23):

$$\begin{aligned}\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle &= \lim_{t_2\to\infty}\langle \mathbf{p}'|\hat{U}_I(t_2, 0)|\mathbf{p}^{(+)}\rangle \\ &= \lim_{t_2\to\infty}\langle \mathbf{p}'|e^{i\hat{H}_0 t_2}e^{-i\hat{H}t_2}|\mathbf{p}^{(+)}\rangle \\ &= \lim_{t_2\to\infty} e^{i\left(E_{\mathbf{p}'}-E_{\mathbf{p}}\right)t_2}\langle \mathbf{p}'|\mathbf{p}^{(+)}\rangle.\end{aligned} \tag{7.104}$$

Then we use the Lippmann-Schwinger equation (7.41) for $|\mathbf{p}^{(+)}\rangle$ and have

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \lim_{t_2\to\infty} e^{i\left(E_{\mathbf{p}'}-E_{\mathbf{p}}\right)t_2}\left[\langle \mathbf{p}'|\mathbf{p}\rangle + \frac{1}{E_{\mathbf{p}} - E_{\mathbf{p}'} + i\eta}\langle \mathbf{p}'|\hat{V}|\mathbf{p}^{(+)}\rangle\right]. \tag{7.105}$$

The first term in brackets is nonzero only if the momenta are equal, $\mathbf{p}' = \mathbf{p}$, in which case also the energies are equal, $E_{\mathbf{p}'} = E_{\mathbf{p}}$ and the right-hand side is unaffected by the limit $t_2 \to -\infty$ in the prefactor.

We shall imagine the system to be enclosed in a box of a large volume V (not to be confused with the potential $\hat{V}$). Then the momenta are discrete and the first term is simply

$$\delta_{\mathbf{p}',\mathbf{p}}.$$

It describes the amplitude for the *direct beam* to appear behind the scattering region, containing all the unscattered particles. In front of the second term, the limit $t_2 \to \infty$ in the prefactor is nontrivial. If $E' \neq E$, it oscillates so fast that it can be set equal to zero, by the Riemann-Lebesgue lemma. For $E' = E$ it is identically equal to unity so that

$$\lim_{t_2\to\infty} \frac{e^{i(E'-E)t_2}}{E - E' + i\eta} = \begin{cases} 0, & E' \neq E, \\ -i/\eta, & E' = E. \end{cases} \tag{7.106}$$

It is easy to see that such a property defines a δ-function in the energy:

$$\lim_{t_2\to\infty} \frac{e^{i(E'-E)t_2}}{E - E' + i\eta} = -2\pi\delta(E' - E). \tag{7.107}$$

Indeed, if we integrate the left-hand side over a smooth function $f(E')$ and set

$$E' \equiv E + \xi/t_2, \tag{7.108}$$

then the E'-integral can be rewritten as

$$-\int_{-\infty}^{\infty} d\xi \frac{e^{i\xi}}{\xi - i\eta} f\left(E + \xi/t_2\right). \tag{7.109}$$

In the limit of large t_2, the function $f(E)$ can be taken out of the integral and the contour of integration can then be closed in the upper half-plane giving $-2\pi i$, as the right-hand side of (7.107) would do. The δ-function ensures the conservation of energy in the scattering process.

It is customary to introduce the quantity

$$\langle \mathbf{p}'|R|\mathbf{p}\rangle \equiv \langle \mathbf{p}'|\hat{V}|\mathbf{p}^{(+)}\rangle \tag{7.110}$$

as the *reactance matrix* or *R-matrix*, so that the S-matrix decomposes into a direct beam contribution plus an energy conserving scattering contribution as follows

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'|\mathbf{p}\rangle - 2\pi i\delta(E' - E)\langle \mathbf{p}'|R|\mathbf{p}\rangle. \tag{7.111}$$

In terms of R, the Lippmann-Schwinger equation (7.41) reads

$$|\psi^{(+)}(0)\rangle = |\psi_{\rm in}\rangle + \frac{1}{E - \hat{H}_0 + i\eta} R|\psi_{\rm in}(0)\rangle, \tag{7.112}$$

The Lippmann-Schwinger equation implies that the R matrix obeys an integral equation

$$R = \hat{V} + \hat{V}\frac{1}{E - \hat{H}_0 - i\eta}R. \tag{7.113}$$

The square of the matrix elements of the R matrix gives directly the *differential cross sections* observed in experiment. The differential cross section $d\sigma/d\Omega$ is defined by the probability rate $d\dot{P}(t)$ for an incoming particle to be scattered into solid angle $d\hat{\Omega} = d\cos\theta d\varphi$ around the direction $\hat{\mathbf{p}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, divided by the incoming particle current density j, which is the number of incoming particles per area and second of the incoming beam:

$$\frac{d\sigma}{d\Omega} = \frac{d\dot{P}(t)}{d\Omega}\frac{1}{j}. \tag{7.114}$$

The differential cross section has the dimension of an area. The total rate of scattered particles is given by

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega}. \tag{7.115}$$

The scattering amplitudes are often analyzed separately for each angular momentum of the scattered particles. The R-matrix $\langle \mathbf{p}'|R|\mathbf{p}\rangle$ in Eq. (7.110) has for equal incoming and outgoing energies $E_{\mathbf{p}'} = E_{\mathbf{p}}$, i.e., $|\mathbf{p}'| = |\mathbf{p}| = p$ an expansion

$$\langle \mathbf{p}'|R|\mathbf{p}\rangle \;=\; \sum_{l=0}^{\infty} R_l(p) \sum_{m=-l}^{l} Y_{lm}(\hat{\mathbf{p}}')Y_{lm}(\hat{\mathbf{p}}), \tag{7.116}$$

where $Y_{lm}(\hat{\mathbf{p}})$ are the spherical harmonics (3D.1) associated with the momentum direction $\hat{\mathbf{p}}$:

$$Y_{lm}(\hat{\mathbf{p}}) = Y_{lm}(\theta,\varphi) \equiv (-1)^m \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\varphi}. \tag{7.117}$$

They satisfy the orthogonality relation (3D.3), which we shall write in the form

$$\int d^2\hat{\mathbf{p}}\, Y^*_{l'm'}(\hat{\mathbf{p}})Y_{lm}(\hat{\mathbf{p}}) = \delta_{l'l}\delta_{m'm}, \tag{7.118}$$

where $\int d^2\hat{\mathbf{p}}$ denotes the integral over the surface of a unit sphere:

$$\int d^2\hat{\mathbf{p}} \equiv \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\varphi. \tag{7.119}$$

It is useful to view the spherical harmonics as matrix elements of eigenstates $|l,m\rangle$ of angular momentum [recall (3.781)] with localized states $|\hat{\mathbf{p}}\rangle$ on the unit sphere:

$$\langle \hat{\mathbf{p}}|l,m\rangle \equiv Y_{lm}(\hat{\mathbf{p}}). \tag{7.120}$$

The latter are orthogonal:

$$\langle \hat{\mathbf{p}}'|\hat{\mathbf{p}}\rangle = \delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}), \tag{7.121}$$

where $\delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}})$ is the δ-function on a unit sphere:

$$\delta^{(2)}(\hat{\mathbf{p}}' - \hat{\mathbf{p}}) \equiv \delta(\cos\theta' - \cos\theta)\delta(\varphi' - \varphi). \tag{7.122}$$

With the help of the addition theorem

$$\frac{2l+1}{4\pi}P_l(\cos\Delta\vartheta) = \sum_{m=-l}^{l} Y_{lm}(\theta',\varphi')Y^*_{lm}(\theta,\varphi), \tag{7.123}$$

the *partial-wave expansion* (7.116) becomes

$$\langle \mathbf{p}'|R|\mathbf{p}\rangle \;=\; \sum_{l=0}^{\infty} R_l(p)\frac{2l+1}{4\pi}P_l(\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}}). \tag{7.124}$$

where $P_l(\cos\theta) \equiv P_l^0(\cos\theta)$ are the Legendre polynomials (3D.7).

A similar expansion of the S-matrix (7.111) requires expanding the scalar product $\langle \mathbf{p}'|\mathbf{p}\rangle = \delta_{\mathbf{p}',\mathbf{p}}$ into partial waves. In a large volume V, we replace this by $(2\pi)^3\delta^{(3)}(\mathbf{p}'-\mathbf{p})/V$. The δ-function is decomposed into a directional and a radial part

$$\delta_{\mathbf{p}',\mathbf{p}} = \frac{(2\pi)^3}{V}\delta^{(3)}(\mathbf{p}'-\mathbf{p}) = \delta^{(2)}(\hat{\mathbf{p}}'-\hat{\mathbf{p}})\frac{(2\pi)^3}{V}\frac{1}{p^2}\delta(p'-p). \tag{7.125}$$

The directional δ-function on the right-hand side has a partial-wave expansion which is, in fact, the completeness ralation (3C.1) for the states $|l,m\rangle$,

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} |l,m\rangle\langle l,m| = 1, \tag{7.126}$$

evaluated between the localized states $|\hat{\mathbf{p}}\rangle$ on the unit sphere. Using the matrix elements (7.120) and the orthogonality relation (7.121), we find from (7.126):

$$\delta^{(2)}(\hat{\mathbf{p}}'-\hat{\mathbf{p}}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta',\varphi')Y^*_{lm}(\theta,\varphi). \tag{7.127}$$

The radial part of (7.125) δ-function can be rewritten as

$$\frac{(2\pi)^3}{V}\frac{1}{p^2}\delta(p'-p) = \frac{(2\pi)^3}{V}\frac{1}{p^2}\frac{dE}{dp}\delta(E'-E) = \frac{1}{\rho_E}\delta(E'-E), \tag{7.128}$$

where

$$\rho_E \equiv \frac{V}{(2\pi)^3}\frac{p^2}{dE/dp} \tag{7.129}$$

is the density of energy levels on the E-axis in a large volume V. It allows us to rewrite the sum over all momentum states as follows:

$$\sum_{\mathbf{p}} = \int\frac{d^3pV}{(2\pi)^3} = \int d^2\hat{\mathbf{p}}\int dE\,\rho_E. \tag{7.130}$$

Thus we find the expansion

$$\langle \mathbf{p}'|\mathbf{p}\rangle = \delta_{\mathbf{p}',\mathbf{p}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\hat{\mathbf{p}}')Y_{lm}(\hat{\mathbf{p}})\frac{1}{\rho_E}\delta(E'-E). \tag{7.131}$$

In a partial-wave expansion for the S-matrix (7.111), the overall δ-function for the energy conservation is conventionally factored out and one writes:

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \frac{1}{\rho_E}\delta(E'-E)\sum_{l=0}^{\infty} S_l(p) \sum_{m=-l}^{l} Y_{lm}(\hat{\mathbf{p}}')Y_{lm}(\hat{\mathbf{p}}), \tag{7.132}$$

The relation between the *partial-wave scattering amplitudes* $S_l(p)$ and those of the R-matrix is

$$S_l(p) = 1 - 2\pi i \rho_E R_l(p). \tag{7.133}$$

The potential scattering under consideration is purely elastic. For such processes, the unitarity property (7.51) of the S-matrix implies

$$\int \frac{d^3p''V}{(2\pi)^3}\langle \mathbf{p}'|\hat{S}^\dagger|\mathbf{p}''\rangle\langle \mathbf{p}''|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'|\mathbf{p}\rangle. \tag{7.134}$$

Inserting the partial-wave decomposition (7.132) and using (7.130) as well as the orthogonality relation (7.118), we derive from this the unitarity property of the partial waves of elastic scattering $S_l^*(p)S_l(p) = 1$, implying that $S_l(p)$ is a pure phase factor:

$$S_l(p) = e^{2i\delta_l(p)}. \tag{7.135}$$

For the amlitudes $R_l(p)$ in (7.133) this implies

$$R_l(p) = -\frac{1}{\pi\rho_E}e^{i\delta_l(p)}\sin\delta_l(p). \tag{7.136}$$

The quantities $\delta_l(p)$ are the *phase shifts* observed in the scattered waves of angular momentum l with respect to the incoming waves.

In order to show this we use the expansion formula

$$e^{iz\cos\vartheta} = \sqrt{\frac{\pi}{2z}}\sum_{l=0}^{\infty} i^l J_{l+1/2}(z)(2l+1)P_l(\cos\vartheta), \tag{7.137}$$

where the Bessel functions $J_{l+1/2}(z)$ can be expressed in terms of spherical Bessel functions $j_l(z)$ as

$$J_{l+1/2}(z) = \sqrt{\frac{2z}{\pi}}j_l(z), \tag{7.138}$$

to expand the incoming free-particle wave

$$\langle \mathbf{x}|\mathbf{p}\rangle = \frac{1}{\sqrt{V}}e^{i\mathbf{p}\mathbf{x}} = \sum_{l=0}^{\infty}\psi_l(pr)\sum_{m=-l}^{l}Y_{lm}(\hat{\mathbf{x}})Y_{lm}(\hat{\mathbf{p}}) = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\psi_l(pr)P_l(\hat{\mathbf{x}}\cdot\hat{\mathbf{p}}), \tag{7.139}$$

where $r \equiv |\mathbf{x}|$, with the partial waves

$$\psi_l(pr) = \frac{1}{\sqrt{V}}i^l 4\pi j_l(pr). \tag{7.140}$$

Far from the scattering region, the spherical Bessel functions have the asymptotic behavior

$$j_l(pr) \to \frac{\sin(pr - \pi l/2)}{kr}, \tag{7.141}$$

implying for the partial waves

$$\psi_l(pr) = \frac{1}{\sqrt{V}} i^l 4\pi \frac{\sin(pr - \pi l/2)}{pr}. \tag{7.142}$$

We shall now calculate the asymptotic form of the outgoing waves. Inserting (7.140) into the second term of the Lippmann-Schwinger equation (7.112), we calculate in configuration space the scattered wave

$$\langle \mathbf{x}|\mathbf{p}\rangle^{\rm sc} = \int \frac{d^3p'V}{(2\pi)^3} \langle \mathbf{x}|\mathbf{p}'\rangle\langle \mathbf{p}'|R|\mathbf{p}\rangle. \tag{7.143}$$

After partial wave decompositions (7.132) and (7.139), we see that

$$\int \frac{d^3p'V}{(2\pi)^3}\langle \mathbf{x}|\mathbf{p}'\rangle\langle \mathbf{p}'|R|\mathbf{p}\rangle = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\hat{\mathbf{x}}')Y_{lm}(\hat{\mathbf{p}})\frac{V}{(2\pi)^3}\int_0^\infty 4\pi p'^2 dp' \frac{j_l(p'r)R_l(p)}{E-E'+i\eta}, \tag{7.144}$$

so that the scattered partial waves are

$$\psi_l^{\rm sc}(pr) = \frac{1}{\sqrt{V}}\frac{4\pi}{(2\pi)^3} i^l \left[j_l(pr) + \int_0^\infty dp'\, p'^2\, \frac{j_l(p'r)R_l(p)}{E-E'+i\eta}\right] \tag{7.145}$$

For large r, we use the asymptotic form (7.142) to write

$$\int dE' \rho_{E'} \frac{j_l(pr)R_l(p)}{E-E'+i\eta} = -\frac{V}{(2\pi)^3}4\pi\int p'^2 dp' \frac{R_l(p)}{E-E'+i\eta}\,\frac{e^{i(p'r-\pi l/2)} - e^{-i(p'r-\pi l/2)}}{2ip'r}. \tag{7.146}$$

The integral is very fast oscillating in p' and can receive a nonzero contribution only from a neighborhood of the pole term in the enery.[4] There we can approximate

$$E - E' \approx \frac{dE}{dp}(p-p')\rho_E \tag{7.147}$$

and $p' \approx p$ in all terms except for the fast oscillating exponential. The ensuing integral

$$\frac{1}{dE/dp}p^2 \int dp' \frac{1}{p-p'+i\eta}\,\frac{e^{i(p'r-\pi l/2)} - e^{-i(p'r-\pi/2l)}}{2ipr} \tag{7.148}$$

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[4] This is a conequence of the *Riemann-Lebesgue lemma*. See Chapter 1 of E.C. Titchmarsh, *Introduction to the Theory of the Fourier Integral*, Oxford University Press, Oxford, 1937.

can be extended to the entire p'-axis with a negligible error for large r. The part containing the second exponential is evaluated by closing the contour of integration in the lower half-plane. There the integrand is regular so that the contour can be contracted to a point yielding zero. In the part with the first exponential we close the contour in the upper half-plane and deform it to pick up the pole at $p' = p + i\eta$. Then Cauchy's theorem yields

$$\frac{1}{dE/dp} p^2 \int dp' \frac{1}{p - p' + i\eta} \frac{e^{i(p'r - \pi l/2)} - e^{-i(p'r - \pi/2l)}}{2ipr} = \frac{2\pi p^2}{dE/dp} e^{-i\pi l/2} \frac{e^{ipr}}{2ipr}, \tag{7.149}$$

so that the scattered wave (7.145) becomes

$$\psi_l^{\rm sc}(pr) \xrightarrow{r\to\infty} \frac{1}{\sqrt{V}} \frac{4\pi}{(2\pi)^3} \left[i^l j_l(pr) - 2\pi \rho_E \frac{e^{ipr}}{2pr} \right]. \tag{7.150}$$

Expressing $R_l(p)$ in terms of $S_l(p)$, and using the asymptotic form (7.141) for $j_l(pr)$, we see that (7.150) can be rewritten as

$$\psi_l^{\rm sc}(pr) \xrightarrow{r\to\infty} \frac{1}{\sqrt{V}} \frac{4\pi}{(2\pi)^3} \frac{1}{2ipr} \left[S_l(p) e^{ipr} - (-1)^l e^{-ipr} \right]. \tag{7.151}$$

Inserting the unitary form (7.135) for elastic scattering, this becomes

$$\psi_l^{\rm sc}(pr) \xrightarrow{r\to\infty} \frac{1}{\sqrt{V}} \frac{4\pi}{(2\pi)^3} i^l e^{i\delta_l(p)} \frac{\sin(pr - \pi l/2 + \delta_l(p))}{2pr}. \tag{7.152}$$

This shows that $\delta_l(p)$ is indeed the phase shift of the scattered waves with respect to the incoming partial waves (7.142).

At small momenta, the $l = 0$ (s-wave) phase shifts usually dominate the scattering process. For short-range potentials, they may be parametrized as

$$p \cot \delta_0 = \frac{1}{a} + \frac{1}{2} r_{\rm eff} p^2 + \dots\ . \tag{7.153}$$

where a is called the *scattering length*, wheras $r_{\rm eff}$ is called the *effective range* of the scattering process. In the limit $p \to 0$, only the scattering length survives which goes to zero like

$$\delta_0 \approx ap + \mathcal{O}((ap)^2). \tag{7.154}$$

In this limit,

$$R_0(p) \to -\frac{(2\pi)^3}{V} \frac{a}{\pi M}, \tag{7.155}$$

so that

$$\langle \mathbf{p}' | R | \mathbf{p} \rangle \to -2\pi V \frac{a}{M}. \tag{7.156}$$

The time-dependent version of the incoming wave functions (7.139) is

$$\langle \mathbf{x} | \mathbf{p}, t \rangle = \psi_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{V}} e^{-i(E_0 t - \mathbf{p}\mathbf{x})}. \tag{7.157}$$

The associated incoming current density is

$$\mathbf{j} = \frac{1}{2Mi}\psi^\dagger(\mathbf{x},t)\overleftrightarrow{\boldsymbol{\nabla}}\psi(\mathbf{x},t) = \frac{1}{V}\frac{\mathbf{p}}{M} = \frac{1}{V}\mathbf{v}, \tag{7.158}$$

the factor $1/V$ reflecting the normalization $\langle\mathbf{p}'|\mathbf{p}\rangle = \delta_{\mathbf{p}',\mathbf{p}}$ of one particle per total volume. In order to find the rate of outgoing particles, we differentiate the probability for $t_0 \to -\infty$,

$$\begin{aligned}\frac{dP(t)}{dt} &= \frac{d}{dt}|\langle\mathbf{p}'|\hat{U}_I(t,t_0)|\mathbf{p}\rangle|^2 = \frac{d}{dt}\langle\mathbf{p}'|\hat{U}_I(t,t_0)|\mathbf{p}\rangle\langle\mathbf{p}'|\hat{U}_I(t,t_0)|\mathbf{p}\rangle^* \\ &= 2\mathrm{Im}\left\{\langle\mathbf{p}'|\hat{V}_I(t)\hat{U}_I(t,t_0)|\mathbf{p}\rangle\langle\mathbf{p}'|\hat{U}_I(t,t_0)|\mathbf{p}\rangle^*\right\} \\ &= 2\mathrm{Im}\left\{\langle\mathbf{p}'|\hat{V}_I(t)\hat{U}_I(t,0)\hat{U}_I(0,t_0)\rangle|\mathbf{p}\rangle\langle\mathbf{p}'|\hat{U}_I(t,0)\hat{U}_I(0,t_0)\mathbf{p}\rangle^*\right\} \\ &= 2\mathrm{Im}\left\{\langle\mathbf{p}'|\hat{V}_I(t)\hat{U}_I(t,0)|\mathbf{p}^{(+)}\rangle\langle\mathbf{p}'|\hat{U}_I(t,0)|\mathbf{p}^{(+)}\rangle^*\right\}.\end{aligned} \tag{7.159}$$

Inserting the explicit time dependence of $\hat{V}_I$ and $\hat{U}_I$ and using the fact that $\hat{H}_0$ on $|\mathbf{p}\rangle$ and $\hat{H}$ on $|\mathbf{p}^{(+)}\rangle$ have the same energy eigenvalues, this becomes

$$\begin{aligned}\frac{dP(t)}{dt} &= 2\mathrm{Im}\left\{\langle\mathbf{p}'|e^{i\hat{H}_0t}Ve^{-i\hat{H}_0t}e^{i\hat{H}_0t}e^{-i\hat{H}t}|\mathbf{p}^{(+)}\rangle\langle\mathbf{p}'|e^{i\hat{H}_0t}e^{-i\hat{H}t}|\mathbf{p}^{(+)}\rangle^*\right\} \\ &= 2\mathrm{Im}\left\{\langle\mathbf{p}'|V|\mathbf{p}^{(+)}\rangle\langle\mathbf{p}'|\mathbf{p}^{(+)}\rangle^*\right\} \\ &= 2\langle\mathbf{p}'|\mathbf{p}\rangle\ \mathrm{Im}\,\langle\mathbf{p}'|R|\mathbf{p}\rangle + 2\mathrm{Im}\,\frac{1}{E-E'-i\eta}|\langle\mathbf{p}'|R|\mathbf{p}\rangle|^2 \\ &= 2\langle\mathbf{p}'|\mathbf{p}\rangle\ \mathrm{Im}\,\langle\mathbf{p}|R|\mathbf{p}\rangle + 2\pi\delta(E-E')|\langle\mathbf{p}'|R|\mathbf{p}\rangle|^2.\end{aligned} \tag{7.160}$$

The first term gives the rate of the transmitted particles in the direct beam. The second term gives the rate of scattered particles. If we collect the scattered particles of all final momenta in a sum $\sum_{\mathbf{p}'} = \int d^3pV/(2\pi)^3$ we find the total probability rate

$$\frac{dP}{dt} = \int\frac{d^3p'V}{(2\pi)^3}\,2\pi\delta(E'-E)|\langle\mathbf{p}'|R|\mathbf{p}\rangle|^2. \tag{7.161}$$

There exists a simple mnemonic rule for deriving this formula. The probability for a particle to go from the initial to the final state is given by the absolute square of the scattering amplitude (7.111):

$$P = |\langle\mathbf{p}'|\hat{S}|\mathbf{p}\rangle|^2. \tag{7.162}$$

Excluding the direct beam, this is equal to

$$P = |2\pi\delta(E'-E)\langle\mathbf{p}'|R|\mathbf{p}\rangle|^2. \tag{7.163}$$

Imagining the world to exist only for a finite time T, the δ-function in energy at zero argument is finite:

$$\delta(E)|_{E=0} = \left.\int_{-T/2}^{T/2}\frac{dt}{2\pi}e^{iEt}\right|_{E=0} = \frac{T}{2\pi}. \tag{7.164}$$

Thus we can write (7.163) as

$$P = T\, 2\pi\delta(E' - E)|\langle \mathbf{p}'|R|\mathbf{p}\rangle|^2. \tag{7.165}$$

Multiplying this by the phase space volume we find the probability rate

$$\frac{dP}{dt} = \int \frac{d^3p'V}{(2\pi)^3}\, 2\pi\delta(E' - E)|\langle \mathbf{p}'|R|\mathbf{p}\rangle|^2, \tag{7.166}$$

leading directly to Eq. (7.161). This formula is written in natural units with $c = \hbar = 1$. In proper physical units, the right-hand side carries a factor $1/\hbar$, and is known as Fermi's *golden rule.*

The phase space integral can be split into an integral over the final energy and the final solid angle $d\Omega = d\theta d\varphi$. For nonrelativistic particles, this goes as follows

$$\begin{aligned} \int \frac{d^3p}{(2\pi)^3} &= \frac{1}{(2\pi)^3}\int d\Omega \int_0^\infty \frac{dp^2}{2} p \\ &= \frac{M}{(2\pi)^3}\int d\Omega \int_0^\infty dE\, p. \end{aligned} \tag{7.167}$$

The energy integral removes the δ-function in (7.160) and we can identify the differential cross section as

$$\frac{d\sigma}{d\Omega} = \frac{Mp}{(2\pi)^3} 2\pi |R_{\mathbf{p}'\mathbf{p}}|^2 \frac{1}{j}, \tag{7.168}$$

where we have set

$$\langle \mathbf{p}'|R|\mathbf{p}\rangle \equiv R_{\mathbf{p}'\mathbf{p}}, \tag{7.169}$$

for brevity. Inserting $j = p/MV$ from (7.157) this becomes

$$\frac{d\sigma}{d\Omega} = \frac{M^2V^2}{(2\pi)^2}|R_{\mathbf{p}'\mathbf{p}}|^2. \tag{7.170}$$

If the scattered particle moves relativistically, we have to replace M in (7.167) by $E = \sqrt{p^2 + M^2}$ inside the momentum integral, so that

$$\begin{aligned} \int \frac{d^3p}{(2\pi)^3} &= \frac{1}{(2\pi)^3}\int d\Omega \int_0^\infty dp\, p^2 \\ &= \frac{1}{(2\pi)^3}\int d\Omega \int_M^\infty dE\, E\, p. \end{aligned} \tag{7.171}$$

Also in the relativistic case, the initial current is not proportional to p/M but to the relativistic velocity $v = p/E$ so that

$$j = \frac{1}{V}\frac{p}{E}. \tag{7.172}$$

Hence the cross section becomes

$$\frac{d\sigma}{d\Omega} = \frac{E^2V^2}{(2\pi)^2}|R_{\mathbf{p}'\mathbf{p}}|^2. \tag{7.173}$$

To lowest order in the interaction strength,

$$R_{\mathbf{p}'\mathbf{p}} \approx V_{\mathbf{p}'\mathbf{p}} \tag{7.174}$$

where

$$V_{\mathbf{p}'\mathbf{p}} \equiv \langle \mathbf{p}'|V(\mathbf{x})|\mathbf{p}\rangle = \frac{1}{V}\int d^3x e^{i(\mathbf{p}'-\mathbf{p})\mathbf{x}}V(\mathbf{x}), \tag{7.175}$$

and (7.173) reduces to the so called *Born approximation* (Born 1926)

$$\frac{d\sigma}{d\Omega} \approx \frac{E^2V^2}{(2\pi)^2}|V_{\mathbf{p}'\mathbf{p}}|^2, \tag{7.176}$$

The amplitude whose square is equal to the differential cross section is usually called[5] $f_{\mathbf{p}'\mathbf{p}}$, i.e., one writes

$$\frac{d\sigma}{d\Omega} = |f_{\mathbf{p}'\mathbf{p}}|^2. \tag{7.177}$$

Thus we can identify

$$f \equiv -\frac{EV}{2\pi}R \tag{7.178}$$

where we have chosen the sign to agree with the convention in Landau and Lifshitz' textbook.

Using the partial-wave expansion (7.124), we for f in the nonrelativistic case the well-known expansion

$$f \;=\; \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}f_lP_l(\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}}). \tag{7.179}$$

where

$$f_l = \frac{2\pi}{ik}[S_l(p)-1] = \frac{4\pi}{p}e^{i\delta_l(p)}\sin\delta_l(p). \tag{7.180}$$

As an example, consider a δ-function interaction

$$V(\mathbf{x}) = g\delta^{(3)}(\mathbf{x}). \tag{7.181}$$

Then we find for plane waves the matrix elements

$$\langle \mathbf{p}'|V|\mathbf{p}\rangle = \frac{1}{V}\int d^3x e^{-i\mathbf{p}'\mathbf{x}}\delta^{(3)}(\mathbf{x})e^{i\mathbf{p}\mathbf{x}} = \frac{g}{V}, \tag{7.182}$$

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[5] See for example the textbook by L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Pergamon Press, London, 1965.

so that in Born approximation

$$f = -\frac{E}{2\pi} g. \tag{7.183}$$

Since g has the dimension energy length^3, f has the dimension length as it should to make the cross section an area seen by the incoming beam.

For the δ-function potential, it is instructive to try and calculate also the next correction to the Born approximation. According to Eq. (7.113), it is given by

$$\begin{aligned} R_{\mathbf{p}'\mathbf{p}} &= V_{\mathbf{p}'\mathbf{p}} + \int \frac{d^3p''V}{(2\pi)^3} V_{\mathbf{p}'\mathbf{p}''} \frac{1}{E - E(\mathbf{p}'') + i\eta} V_{\mathbf{p}''\mathbf{p}} + \dots \\ &= V \left[g + g^2 \int \frac{d^3p''}{(2\pi)^3} \frac{1}{E - E(\mathbf{p}'') + i\eta} + \dots \right]. \end{aligned} \tag{7.184}$$

Thus, for zero incoming energy E, the coupling constant g is effectively replaced by

$$g_R = g + g^2 \int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta}, \tag{7.185}$$

and the R-matrix has the isotropic value

$$R_{\mathbf{p}'\mathbf{p}} \overset{p=0}{=} V\, g_R. \tag{7.186}$$

The integral on the right-hand side diverges. A finite result can be obtained by assuming the initial g as being infinitesimal small such as to compensate for the divergence. We are confronted here for the first time with a renormalization problem typical for quantum theories with local interactions. The systematic treatment of this problem will be presented in Chapters 7 and 8.

Due to the simplicity of the δ-function potential, it is possible to find solve the *Lippmann-Schwinger equation* (7.41) exactly and find the full scattering amplitude (7.184). For zero energy, the expression turns out to continue as a geometric series

$$g_R = g + g^2 \int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta} + g^3 \left[\int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta} \right]^2 + \dots . \tag{7.187}$$

This can be summed up to the relation

$$\frac{1}{g_R} = \frac{1}{g} - \int \frac{d^3p}{(2\pi)^3} \frac{1}{E(\mathbf{p}) - i\eta}. \tag{7.188}$$

Inserting (7.186) into (7.156) we see that the renormalized coupling determines the scattering length as

$$a = \frac{M}{2\pi} g_R. \tag{7.189}$$

In quantum field theory, the target is usually not a fixed potential at the origin but a proper particle which can recoil, so that the incoming state consists of two particles with momenta $\mathbf{p}_1$ and $\mathbf{p}_2$. If the scattering is elastic between two identical particles, relation (7.189) changes to

$$a = \frac{M}{4\pi} g_R. \tag{7.190}$$

Usually, the final state has two or more particles leaving the interaction zone. The interaction energy is an integral over some local interaction density

$$\hat{V} = \int d^3x \, \hat{\mathcal{H}}_{\rm int}(x), \tag{7.191}$$

integrated over all space at a fixed time $x_0 = t = 0$. In this case, the matrix elements of the potential factorizes as

$$\langle \mathbf{p}'|\hat{V}|\mathbf{p}\rangle = \int d^3x \, \langle \mathbf{p}'|e^{i\hat{\mathbf{p}}\mathbf{x}}\hat{\mathcal{H}}_{\rm int}(0)e^{-i\hat{\mathbf{p}}\mathbf{x}}|\mathbf{p}\rangle = V\delta_{\mathbf{p}'\,\mathbf{p}}\langle \mathbf{p}'|\hat{\mathcal{H}}_{\rm int}(0)|\mathbf{p}\rangle, \tag{7.192}$$

where $\mathbf{p}$ and $\mathbf{p}'$ are the sum over all initial and final momenta, respectively. Thus the matrix elements of always carry a $V\delta_{\mathbf{p}'\,\mathbf{p}}$ factor ensuring total momentum conservation. The same thing is true for the reactance matrix $R_{\mathbf{p}'\mathbf{p}}$. This factor is customarily removed by defining the so-called *t-matrix*

$$R_{\mathbf{p}'\mathbf{p}} = V\delta_{\mathbf{p}'\,\mathbf{p}} \, t_{\mathbf{p}'\mathbf{p}}. \tag{7.193}$$

The Born approximation is now

$$t_{\mathbf{p}'\mathbf{p}} \approx \langle \mathbf{p}'|\hat{\mathcal{H}}_{\rm int}(0)|\mathbf{p}\rangle. \tag{7.194}$$

Replacing the Kronecker δ for momentum conservation by its continuum limit,

$$\delta_{\mathbf{p}'\,\mathbf{p}} \to \frac{(2\pi)^3}{V}\delta^{(3)}(\mathbf{p}' - \mathbf{p}),$$

we can write (7.193) as

$$R_{\mathbf{p}'\mathbf{p}} = (2\pi)^3\delta^{(3)}(\mathbf{p}' - \mathbf{p}) \, t_{\mathbf{p}'\mathbf{p}}, \tag{7.195}$$

i.e., the matrix elements (7.111) of the S-matrix become

$$\langle \mathbf{p}'|\hat{S}|\mathbf{p}\rangle = \langle \mathbf{p}'|\mathbf{p}\rangle - i(2\pi)^4\delta^{(4)}(p' - p) \, t_{\mathbf{p}'\mathbf{p}}. \tag{7.196}$$

In a world of a finite volume V existing for a finite time T, the probability of going from an initial state $\mathbf{p}$ to e final state $\mathbf{p}'$ is given by the absolute square of (7.196). In analogy to (7.164) we have

$$\delta^{(4)}(p)\big|_{p=0} = \int \frac{d^4p}{(2\pi)^4} e^{ipx}\bigg|_{p=0} = \frac{TV}{(2\pi)^4}, \tag{7.197}$$

so that we obtain the transition rate [compare (7.165)] Thus we can write (7.163) as

$$P = TV(2\pi)^4\delta^{(4)}(p' - p)|t_{\mathbf{p}'\mathbf{p}}|^2. \tag{7.198}$$

This has to be summed over all final particle states, and we obtain the rate.

$$\frac{dP}{dt} = V \sum_{\text{final states}} (2\pi)^4\delta^{(4)}(p' - p)|t_{\text{fi}}|^2. \tag{7.199}$$

We have changed the notation for the t-matrix $t_{\mathbf{p}'\mathbf{p}}$ and written it as t_{fi} to emphasize the validity for a more general initial state $|\text{i}\rangle$ and a larger variety of possible final states $|\text{f}\rangle$.

If the particles $1', 2', \dots, n'$ leave the interaction zone, the sum over all final states in a volume V consists of an integral over the phase space

$$\sum_{\mathbf{p}'_1, \mathbf{p}'_2, \dots} = \int \frac{d^3p'_1}{(2\pi)^3} \int \frac{d^3p'_2}{(2\pi)^3} \cdots \int \frac{d^3p'_n}{(2\pi)^3}, \tag{7.200}$$

and (7.199) becomes

$$\frac{dP}{dt} = V^n \int \frac{d^3p'_1}{(2\pi)^3} \int \frac{d^3p'_2}{(2\pi)^3} \cdots \int \frac{d^3p'_n}{(2\pi)^3} \delta^{(4)}(p' - p)|t_{\text{fi}}|^2, \tag{7.201}$$

where $p = p_1 + p_2$ and $p' = p'_1 + p'_2 + \ldots + p'_n$. By dividing out the current density of the incoming particles j, we find from this the cross section.

$$\sigma = \frac{dP}{dt}\frac{1}{j}. \tag{7.202}$$

By omitting some of the final-state integrations, we may extract from this any desired differential cross section.

7.3.1 Center-of-Mass Scattering Cross Section

Let us assume the collision to take place in the center-of-mass frame with zero total momentum and $\mathbf{p} = \mathbf{p}_1 = -\mathbf{p}_2$ and a total energy E_{CM}. Then the δ-function fixes $\mathbf{p}' = \mathbf{p}'_1 = -\mathbf{p}'_2$ and the equality of the total energies before and after the collision:

$$E'_1 + E'_2 = E_1 + E_2 = E_{\text{CM}}. \tag{7.203}$$

In order to be more explicit we have to distinguish the case of nonrelativistic and relativistic particles. It is useful to treat the relativistic case first and obtain the nonrelativistic result by going to the limit of small velocities. In the relativistic case with initial momenta $\mathbf{p} = \mathbf{p}_1 = -\mathbf{p}_2$ and energies

$$E_{1,2} = \sqrt{p^2 + M_{1,2}^2}, \quad E'_{1,2} = \sqrt{p'^2 + {M'_{1,2}}^2} \tag{7.204}$$

the δ-functions for the total energy reads, in the center-of-mass frame,

$$\delta\left(\sqrt{p'^2+M_1'^2}+\sqrt{p'^2+M_2'^2}-E_{\rm CM}\right). \tag{7.205}$$

This vanishes unless p' makes the argument zero which happens at

$$p'=p'_{\rm CM}=\frac{1}{2M}I\left(M,M_1',M'_{,2}\right) \tag{7.206}$$

where

$$I(M,M_1,M_2)\equiv\sqrt{M^2-(M_1+M_2)^2}\sqrt{M^2-(M_1-M_2)^2} \tag{7.207}$$

and

$$M=E_{\rm CM} \tag{7.208}$$

is the total mass in the center-of-mass frame, often denoted by $\sqrt{s}$. The individual energies of the two particles are

$$\begin{aligned} E_{1,2} &= \sqrt{p_{\rm CM}^2-M_{1,2}^2}=\frac{1}{2}\left[M^2\pm\left(M_1^2-M_2^2\right)\right], \\ E'_{1,2} &= \sqrt{p_{\rm CM}^2-M'^2_{1,2}}=\frac{1}{2M}\left[M^2\pm\left(M_1'^2-M_2'^2\right]\right). \end{aligned} \tag{7.209}$$

To evaluate the momentum integral over the δ-function (7.205), we use the formula

$$\delta\left(f(p')-f(p'_{\rm CM})\right)=\left[f'(p')\right]^{-1}\delta(p'-p'_{\rm CM}) \tag{7.210}$$

to write

$$\begin{aligned} &\delta\left(\sqrt{p'^2+M_1'^2}+\sqrt{p'^2+M_2'^2}-E_{\rm CM}\right) \\ &\quad=\left[\left(\partial/\partial p'\right)\left(E_1'+E_2'\right)\right]^{-1}\delta(p'-p'_{\rm CM}) \\ &\quad=\frac{E_1'E_2'}{p'_{\rm CM}\left(E_1'+E_2'\right)}\delta(p'-p'_{\rm CM})=\frac{E_1'E_2'}{p'_{\rm CM}E_{\rm CM}}\delta(p'-p'_{\rm CM}). \end{aligned} \tag{7.211}$$

Then we obtain from (7.201) the total rate of scattered relativistic particles

$$\frac{dP(t)}{dt}=\frac{V^3}{(2\pi)^2}\frac{p'_{\rm CM}E_1'E_2'}{E_{\rm CM}}\int d\Omega|t_{\rm fi}|^2. \tag{7.212}$$

Since, the t-matrix elements depend, in general, on more than just the initial and final total momenta $\mathbf{p}$ and $\mathbf{p}'$ we have denoted the matrix elements of t between initial and final states by $t_{\rm fi}$.

The initial current density is given by the relative velocity between two incoming particles in the center-of-mass frame [see (7.158) and (7.172)]. Hence

$$j=\left(\frac{p_1}{E_1}-\frac{p_2}{E_2}\right)\frac{1}{V}=\frac{p_{\rm CM}E_{\rm CM}}{E_1E_2}\frac{1}{V}. \tag{7.213}$$

Dividing $dP(t)/dt$ by j as demanded by (7.202) and omitting the integration over the solid angle in (7.212), we obtain the differential cross section in the center of mass:

$$\frac{d\sigma}{d\Omega_{\rm CM}}=\frac{1}{(2\pi)^2}\frac{p'_{\rm CM}}{p_{\rm CM}}\frac{1}{E_{\rm CM}^2}E'_1E'_2E_1E_2V^4|t_{\rm fi}|^2. \tag{7.214}$$

It is useful to realize that the combination of incoming currents and energies $j\times 2VE_1E_2$ is a Lorentz-invariant quantity coinciding with $I(M,m_1,m_2)$ of Eq. (7.207). This follows immediately by inserting (7.206) into (7.213):

$$j=\frac{1}{2VE_1E_2}I(M,m_1,m_2). \tag{7.215}$$

Thus we can write down an explicit formula for the cross section (7.202) any frame of reference:

$$\sigma=V^n\int\frac{d^3p'_1}{(2\pi)^3}\int\frac{d^3p'_2}{(2\pi)^3}\cdots\int\frac{d^3p'_n}{(2\pi)^3}\delta^{(4)}(p'-p)|t_{\rm fi}|^2\frac{2VE_1E_2}{I(M,m_1,m_2)}. \tag{7.216}$$

7.3.2 Laboratory Scattering Cross Section

In most experiments, the directly measure quantity is the laboratory cross section where an initial particle of momenta $p_1=p_{\rm L}$ and energy

$$E_{\rm L}\equiv(E_1)_{\rm Lab}=\sqrt{p_{\rm L}^2+M_1^2} \tag{7.217}$$

hits the particle 2 at rest. Then the incoming current is

$$j=\frac{p_L}{E_LV}=\frac{v_L}{V}, \tag{7.218}$$

rather than (7.213). The cross section of two particles going into two particles in the laboratory is from (7.201) and (7.202):

$$\sigma=\int\frac{d^3p'_1V}{(2\pi)^3}\frac{d^3p'_1V}{(2\pi)^3}(2\pi)^4\delta^{(4)}(\mathbf{p}'-\mathbf{p})|t_{\rm fi}|^2\frac{V}{j} \tag{7.219}$$

The δ-function for the total energy is now

$$\delta\left(\sqrt{p_1'^2+M_1'^2}+\sqrt{p_2'^2+M_2'^2}-E_{\rm L}-M_2\right) \tag{7.220}$$

The momenta p_1' and p_2' are no longer equal which complicates the issue. We would like to express them as functions of the initial energy and the scattering angle $\theta_{\rm L}$. For this some kinematic considerations are necessary.

The total mass introduced in (7.208) is given in a Lorentz invariant way by

$$M^2 = (p_1 + p_2)^2 = M_2^2 + M_2^2 + 2M_2E_{\rm L}. \tag{7.221}$$

Solving this we obtain the invariant expressions

$$\begin{aligned} E_{\rm L} &= \left(M^2 - M_1^2 - M_1^2 - M_2^2\right)/2M_2 \\ p_{\rm L} &= I\left(M, M_1M_2\right)/2M_2. \end{aligned} \tag{7.222}$$

Observe that by inserting the last equation into the frame-independent expression (7.215), we find the correct current (7.218) in the laboratory frame.

The relation between the laboratory and center-of-mass energies is

$$E_{1\rm CM} = \frac{M_2E_{\rm L} + M_1^2}{\sqrt{M_1^2 + M_2^2 + 2E_{\rm L}M_2}}, \tag{7.223}$$

$$E_{2\rm CM} = \frac{M_2E_{\rm L} + M_2^2}{\sqrt{M_1^2 + M_2^2 + 2E_{\rm L}M_2}}. \tag{7.224}$$

The relation between the laboratory the center-of-mass momenta is

$$p_{\rm CM} = p_{\rm L}\frac{M_1}{\sqrt{M_1^2 + M_2^2 + 2E_{\rm L}M_2}}. \tag{7.225}$$

The relation between the scattering angles in the two frames of reference is more involved. To find it, we consider the Lorentz invariant formed from the momentum transfer

$$t \equiv (p_1 - p_1')^2 = M_1^2 + M_1'^3 + 2(\mathbf{p}_1\mathbf{p}_1' - E_1E_1'). \tag{7.226}$$

In either frame, the scattering angles appear in the scalar product $\mathbf{p}_1\mathbf{p}_1' = p_1p_1'\cos\theta$. A calculation in the center-of-mass frame, leads to the formula

$$\begin{aligned} \cos\theta_{\rm CM} &= \frac{1}{2p_{\rm CM}p_{\rm CM}'}(t - M_1^2 - M_1'^2 + 2E_{1\rm CM}E_{1\rm CM}') \\ &= \frac{1}{I(M, M_1, M_2)I(M, M_1', M_2')} \\ &\quad \times[M^4 + M^2(2t - M_1^2 - M_2^2 - M_1'^2 - M_2'^2) + (M_1^2 - M_2^2)(M_1'^2 - M_2'^2)] \end{aligned} \tag{7.227}$$

In the laboratory frame, we take advantage of the fact that $p_2 = (M_2, \mathbf{0})$ and calculate t using energy-momentum conservation as

$$t = (p_2' - p_2) = M_2'^2 + M_2^2 - 2M_2E_{2\rm L}' \tag{7.228}$$

It is convenient to introduce another invariant momentum transfer

$$u \equiv (p_1 - p_2')^2 = (p_1' - p_2)^2 = M_2^2 - M_1'^2 - 2M_2 E_{1\mathrm{L}}'. \tag{7.229}$$

The three invariants are related by

$$s + t + u = M_1^2 + M_2^2 + M_1'^2 + M_2'^2. \tag{7.230}$$

Note that

$$E_{2\mathrm{L}} = \frac{1}{M_2}(M_2^2 + M_2'^2 - t), \tag{7.231}$$

$$E_{1\mathrm{L}}' = \frac{1}{M_2}(M_2^2 + M_1'^2 - u). \tag{7.232}$$

We now evaluate Eq. (7.226) in the laboratory frame and find

$$\begin{aligned} \cos\theta_{\mathrm{L}} \;\; = \;\; & \frac{1}{I(M, M_1, M_2) I(M, M_1', M_2')} \\ & \times [M^4 - M_1^2 - M_2^2)(M_2^2 + M_1'^2 - u) + 2M_2^2(t - M_1^2 - M_1'^2)]. \end{aligned} \tag{7.233}$$

In (7.220) we had to know the momenta p_1', p_2' of the final particles as a function of the initial energy E_L and the scattering angle θ_L. These can now be calculated as follows. From (7.221) we find the invariant M as a function of E_L. This is inserted into (7.234) to obtain the invariant t as a function. Together with (7.230), this fixes the invariant u. Inserted into Eqs. (7.232), we find the final energy E_{1L}', and from energy conservation also E_{2L}'. These determine the final momenta.

It is useful to generalize the definition of the scattering amplitude f of (7.178) (for the scattering of a nonrelativistic particle in an external potential) to the present case of two relativistic particles scattering each other in the center-of-mass frame. We define again f so that

$$\frac{d\sigma}{d\Omega_{\mathrm{CM}}} = |f|^2 \tag{7.234}$$

and see that f has to be identified with

$$f = -\frac{1}{2\pi}\sqrt{\frac{p_{\mathrm{CM}}'}{p_{\mathrm{CM}}}}\frac{1}{E_{\mathrm{CM}}}\sqrt{V^4 E_1' E_2' E_1 E_2}\; t_{\mathrm{fi}}. \tag{7.235}$$

In the case of elastic scattering on a very heavy particle 2, this reduces back to the original definition.

For a more general scattering process in which two particles collide and produce n particles in the final state the production cross section is given by

$$\sigma_{\mathrm{fi}} = \frac{V}{j}\prod_{i=1}^{n}\left[\int \frac{d^3 p_i V}{(2\pi)}\right](2\pi)^4 \delta^{(4)}(p' - p)|t_{\mathrm{fi}}|^2 \tag{7.236}$$

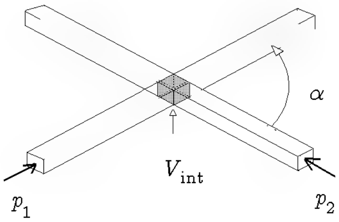

FIGURE 7.1 Geometry of particle beams in a collider. The angle of intersection α is greatly exaggerated. The intersection defines the interaction volume $\hat{V}_{\rm int}$.

with the prefactor $V/j = V^2 E_1 E_2 / p_{\rm CM} E_{\rm CM}$ as given by (7.213),

Scattering processes in a center-of-mass frame can be observed directly in colliding beam experiments. There one has two beams impinging almost with opposite momenta (see Fig. 22.8). If $\hat{V}_{\rm int}$ is the volume of the intersecting zone, the interaction volume and n_1, n_2 are the particle densities in the two beams (particles per unit volume), the relative velocity $v_{\rm rel}$ integrated over the interaction volume is the so-called *luminosity* of the colliding beam:

$$L = v_{\rm rel} \hat{V}_{\rm int} n_1 n_2 = \frac{I(M, m_1, m_2)}{2E_1 E_2} \hat{V}_{\rm int} n_1 n_2. \tag{7.237}$$

The rate of particle scattering is obtained by multiplying the differential cross section $d\sigma/d\Omega_{\rm CM}$ by this quantity:

$$\frac{dN}{dt d\Omega_{\rm CM}} = \frac{d\sigma}{d\Omega_{\rm CM}} L. \tag{7.238}$$

Note that the luminosity increases linearly if the beams are focused upon a smaller area (since $n_1 n_2$ increases like $1/\text{area}^2$ while $\hat{V}_{\rm int}$ increases like area).

7.4 DECAY

The decay rate of an unstable one particle state into two particles is directly given by

$$\Gamma = \frac{d}{dt} P(t) = \frac{V^3}{(2\pi)^2} \frac{p'_{\rm CM} E'_1 E'_2}{M} \int d\Omega |t_{\rm fi}|^2 \tag{7.239}$$

where M is the mass of the initial particle.

7.5 OPTICAL THEOREM

The unitarity of the S-matrix (7.51),

$$\hat{S}\hat{S}^\dagger = \hat{S}^\dagger \hat{S} = 1, \tag{7.240}$$

implies an important theorem for the imaginary part of the diagonal elements of the reaction matrix. Writing

$$S_{\mathrm{fi}} = \delta_{\mathrm{fi}} - (2\pi)^4 \delta^{(4)} \left(p_{\mathrm{f}} - p_{\mathrm{i}}\right) \; i\, t_{\mathrm{fi}} \tag{7.241}$$

we see that

$$-\, i \left(t_{\mathrm{ii}} - t_{\mathrm{ii}}^{\dagger}\right) = -\sum_f t^{\dagger}{}_{\mathrm{if}} (2\pi)^4 \delta^{(4)} \left(p_{\mathrm{f}} - p_{\mathrm{i}}\right) t_{\mathrm{fi}} \tag{7.242}$$

where the sum runs over all possible many particle states. According to Eq. (7.235), the left-hand side is related to the imaginary part of the forward scattering amplitude f_{ii} as follows

$$\frac{2\pi E_{\mathrm{CM}}}{V^2 E_1 E_2} \mathrm{Im}\, f_{\mathrm{ii}} = -\sum_n \prod_{i=1}^{n} \left[\int \frac{d^3 p_{\mathrm{i}} V}{(2\pi)^3}\right] (2\pi)^4 \delta^{(4)} \left(p_{\mathrm{f}} - p_1\right) \left|t_{\mathrm{fi}}\right|^2 \tag{7.243}$$

Now, the right-hand side, if divided by the relative current density $j = p_{\mathrm{CM}} E_{\mathrm{CM}} / E_1 E_2 V$, is equal to $1/V$ times the sum over all cross sections σ_{fi},i.e., it is equal to $-j/V$ times the total cross section $-(j/V)\sigma_{\mathrm{tot}}$ [see (7.219)]. For the forward scattering amplitude f_{ii} this implies the simple relation

$$\frac{2\pi}{p_{\mathrm{CM}}} f_{\mathrm{ii}} = -\sigma_{\mathrm{tot}}. \tag{7.244}$$

This relation is referred to as the *optical theorem* (in reference to a theorem relating the total absorption of light to the imaginary part of the forward-scattering amplitude).

7.6 INITIAL- AND FINAL-STATE INTERACTIONS

Some inelastic scattering and decay processes are caused a weak interaction $\hat{H}_{\mathrm{w}}$ which can be treated in Born approximation, whereas the initial and final states are distorted by a strong interaction $\hat{H}_{\mathrm{s}}$. Suppose the total Hamiltonian contains these interactions additively, i.e.

$$\hat{H} = \hat{H}_0 + \hat{V}_{\mathrm{s}} + \hat{V}_{\mathrm{w}}, \tag{7.245}$$

In specific applications, $\hat{H}_{\mathrm{w}}$ may be *the* weak interaction of beta decay, say, and $\hat{H}_{\mathrm{s}}$ a combination of electromagnetic and strong interactions. Alternatively, $\hat{H}_{\mathrm{w}}$ may be an electromagnetic interaction, and $\hat{H}_{\mathrm{s}}$ the strong interaction.

For time-independent interactions, the Møller operators are given by (7.32) and read explicitly

$$\Omega^{(\pm)} = \hat{U}_I \left(0, \mp\infty\right) = \lim_{t \to \mp\infty} e^{i(\hat{H}_0 + \hat{V}_{\mathrm{w}} + \hat{V}_{\mathrm{s}})t} e^{-i\hat{H}_0 t}, \tag{7.246}$$

The right-hand sides can obviously be decomposed into a product

$$\hat{U}_I \left(0, \mp\infty\right) = \hat{U}_{I\mathrm{w}} \left(0, \mp\infty\right) \hat{U}_{I,\mathrm{s}} \left(0, \mp\infty\right), \tag{7.247}$$

where

$$\hat{U}_{I\text{w}}(0, \mp\infty) = \lim_{t\to\mp\infty} e^{i(\hat{H}_0+\hat{V}_\text{s}+\hat{V}_\text{w})t} e^{-i(\hat{H}_0+\hat{H}_\text{s})t}, \tag{7.248}$$

$$\hat{U}_{I\text{s}}(0, \mp\infty) = \lim_{t\to\mp\infty} e^{i(\hat{H}_0+\hat{V}_\text{s})t} e^{-i\hat{H}_0 t}, \tag{7.249}$$

Thus we can write the Møller operators as

$$\Omega^{(\pm)} = \Omega^{(\pm)}_\text{w}\Omega^{(\pm)}_\text{s}, \tag{7.250}$$

with

$$\Omega^{(\pm)}_\text{w} = \hat{U}_{I\text{w}}(0, \mp\infty), \quad \Omega^{(\pm)}_\text{s} = \hat{U}_{I\text{w}}(0, \mp\infty). \tag{7.251}$$

Unsing this, we can express the scattering amplitude as follows:

$$S_\text{fi} = \langle\text{f}|\hat{U}_{I\text{s}}(\infty, 0)\hat{S}_\text{w}\hat{U}_{I\text{s}}(0, -\infty)|\text{i}\rangle, \tag{7.252}$$

where, in analogy to (7.49),

$$\hat{S}_\text{w} \equiv \hat{U}_{I\text{w}}(\infty, -\infty) = \Omega^{(-)\dagger}_\text{w}\Omega^{(+)}_\text{w}, \tag{7.253}$$

Using the notation

$$|\text{i}(\pm)\rangle \equiv \hat{U}_{I\text{s}}(0, \mp\infty)|\text{i}\rangle = \Omega^{(+)}_\text{w}|\text{i}\rangle, \tag{7.254}$$

in a slight variation of (7.102), the symbols (±) referring now only to the initial- and final-state interactions, the scattering matrix elements become

$$\langle\text{j}|\hat{S}|\text{i}\rangle = \langle\text{j}(-)|\hat{S}_\text{w}|\text{i}(+)\rangle. \tag{7.255}$$

Under the assumption of a weak V_w, we replace $\hat{S}_\text{w}$ by its Born approximation and write

$$\hat{S}_\text{w} \approx -i\int_{-\infty}^{\infty} dt\hat{V}_{I\text{w}}(t), \tag{7.256}$$

where

$$\hat{V}_{I\text{w}}(t) \equiv e^{i(\hat{H}_0+\hat{V}_\text{s}+\hat{V}_\text{w})t}\hat{V}_\text{w}e^{-i(\hat{H}_0+\hat{V}_\text{s})t} \tag{7.257}$$

is the interaction representation of the weak interaction in the presence of the initial- and final-state interactions. The initial and final states are eigenstates of the operator $\hat{H}_0 + \hat{V}_\text{s})$ [see (7.16)]. The integration over t in (7.256) can therefore be done yielding a δ-function of energy conservation [recall the derivation of (7.111)], and we obtain

$$\langle\text{j}|\hat{S}|\text{i}\rangle = \langle\text{j}|\text{i}\rangle - 2\pi i\delta(E' - E)\langle\text{j}(-)|\hat{V}_\text{w}|\text{i}(+)\rangle. \tag{7.258}$$

For a local interaction which is an integral over an interaction density as in Eq. (7.191), we find the modified expression

$$t_{\mathbf{p}'\mathbf{p}} \approx \langle\mathbf{p}'^{(-)}|\hat{\mathcal{H}}_\text{int}(0)|\mathbf{p}^{(+)}\rangle. \tag{7.259}$$

and for the amplitude of multiparticle scattering (7.199), the initial- and final-state interactions are included in the formula

$$t_\text{fi} \approx \langle\text{f}(-)|\hat{\mathcal{H}}_\text{int}(0)|\text{i}(+)\rangle. \tag{7.260}$$

7.7 TESTS OF TIME-REVERSAL VIOLATIONS

For a time-reversal invariant Hamiltonian, the property (5.114) has the consequence that the scattering operator $\hat{S}$ of Eq. (7.49) satisfies

$$\mathcal{T}^\dagger \hat{S} \mathcal{T} = \hat{S}^\dagger. \tag{7.261}$$

To derive observable consequences from this, we first use the properties (5.109) and (5.110) to write down the trivial equality for any matrix element between an initial state $|\mathrm{i}\rangle$ obtained by applying one or more particle creation operators upon the vacuum, and a similar final state $|\mathrm{f}\rangle$:

$$\langle \mathrm{f}|\hat{S}|\mathrm{i}\rangle = \langle \mathrm{f}|\mathbf{1}_A \hat{S}|\mathrm{i}\rangle^*. \tag{7.262}$$

Invoking now time-reversal invariance in the form (7.261), we obtain

$$\langle \mathrm{f}|\hat{S}|\mathrm{i}\rangle = \langle \mathrm{f}|\mathcal{T}^\dagger \hat{S}^\dagger \mathcal{T}|\mathrm{i}\rangle^* = \langle \mathrm{f}_T|\hat{S}^\dagger|\mathrm{i}_T\rangle^* = \langle \mathrm{i}_T|\hat{S}|\mathrm{f}_T\rangle. \tag{7.263}$$

Here $|\mathrm{i}_T\rangle$ denotes the time-reversed of the state $|\mathrm{i}\rangle$, in which all creation operators are replaced by the right-hand sides of (5.104), (5.310), etc. Thus momenta and spin directions are reversed, and there is a phase factor η_T for each particle.

7.7.1 Strong and Electromagnetic Interactions

Strong and electromagnetic interactions are time-reversal invariant. The matrix elements of the scattering operator $\hat{S}$, the scattering amplitudes, satisfies the identity

$$\langle \mathbf{p}_c, s_{3c}; \mathbf{p}_d, s_{3d}|\hat{S}|\mathbf{p}_a, s_{3a}; \mathbf{p}_b, s_{3b}\rangle = \eta\langle -\mathbf{p}_a, -s_{3a}; -\mathbf{p}_b, -s_{3b}|\hat{S}| - \mathbf{p}_c, -s_{3c}; \mathbf{p}_d, s_{3d}\rangle, \tag{7.264}$$

with some phase factor η of unit norm. When calculating the unpolarized cross section we have to sum over the final and average over the initial states. In the center-of-mass frame, the cross section carries phase space factor p'_{CM}/p_{CM}, the ratio of final and initial center-of-mass momenta. It has to be removed to compare the squared amplitudes. Hence we obtain

$$\frac{\dfrac{d\sigma(ab \to cd)}{d\Omega}}{\dfrac{d\sigma(cd \to ab)}{d\Omega}} = \left(\frac{p_{CM}^{cd}}{p_{CM}^{ab}}\right)^2 \frac{(2s_c+1)(2s_d+1)}{(2s_a+1)(2s_b+1)}. \tag{7.265}$$

This is called the *principle of detailed balance*. It is important for the thermal equilibrium of chemical reactions. This equation was used in 1951 to determine the spin of the pion in the reaction in which two protons produce a pion and a deuteron[6]

$$p + p \rightleftharpoons d + \pi^+. \tag{7.266}$$

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[6] R.E. Marshak, Phys. Rev.**82**, 313 (1951); W.B. Cheston, Phys. Rev. **83**, 1118 (1951); R. Durbin, H. Loar, and J. Steinberger, Phys. Rev. **83**, 646 (1951); D.L. Clark, A. Roberts, and R. Wilson, Phys. Rev. **83**, 649 (1951).

The principle of detailed balance says that

$$\frac{\dfrac{d\sigma(\rightarrow)}{d\Omega}}{\dfrac{d\sigma(\leftarrow)}{d\Omega}}=\frac{3}{4}\frac{q_\pi^2(2s_\pi+1)}{p_p^2}. \tag{7.267}$$

This relation was satisfied with $s_\pi=0$.

7.7.2 Selection Rules in Weak Interactions

Consider a one-particle state $|\mathrm{i}\rangle$ prepared by strong and electromagnetic interactions, which decays into a several-particle state $|b\rangle$ via weak interactions. Let $\hat{\mathcal{O}}$ be an observable wich changes sign under time reversal:

$$\hat{\mathcal{O}}_T=-\hat{\mathcal{O}}. \tag{7.268}$$

Consider the expectation value of $\hat{\mathcal{O}}$ a long time after the decay. It is given by

$$\langle\hat{\mathcal{O}}\rangle=\langle\mathrm{i}|\hat{U}(-\infty,\infty)\hat{\mathcal{O}}\hat{U}(\infty,-\infty)|\mathrm{i}\rangle=\langle\mathrm{i}|\hat{S}^\dagger\hat{\mathcal{O}}\hat{S}|\mathrm{i}\rangle. \tag{7.269}$$

Using the antiunitarity of the time-reversal operator as expressed by Eq. (5.109) and (5.110), the right-hand side can be rewritten as

$$\langle\mathrm{i}|\hat{S}^\dagger\hat{\mathcal{O}}\hat{S}|\mathrm{i}\rangle=\langle\mathrm{i}|\mathbf{1}_A\hat{S}^\dagger\hat{\mathcal{O}}\hat{S}|\mathrm{i}\rangle^*=\langle\mathrm{i}|\mathcal{T}^\dagger\mathcal{T}\hat{S}^\dagger\hat{\mathcal{O}}\hat{S}|\mathrm{i}\rangle^*. \tag{7.270}$$

Time-reversal invariance (7.261) brings this to

$$\langle\mathrm{i}|\mathcal{T}^\dagger\hat{S}\hat{\mathcal{O}}_T\hat{S}^\dagger\mathcal{T}|\mathrm{i}\rangle^*=\langle\mathrm{i}_T|\hat{S}\hat{\mathcal{O}}_T\hat{S}^\dagger|\mathrm{i}_T\rangle^*. \tag{7.271}$$

Since $\hat{\mathcal{O}}$ was assumed to be an observable, the expectation is real, and we can drop the complex conjugation at the end. This leaves us with the relation

$$\langle\hat{\mathcal{O}}\rangle=\langle\mathrm{i}|\hat{S}^\dagger\hat{\mathcal{O}}\hat{S}|\mathrm{i}\rangle=\langle\mathrm{i}_T|\hat{S}\hat{\mathcal{O}}_T\hat{S}^\dagger|\mathrm{i}_T\rangle. \tag{7.272}$$

If the decay is very slow, the scattering operator can ne replaced by its Born approximantion

$$\hat{S}\approx\hat{S}_B\equiv i\int_{-\infty}^{\infty}dt\hat{V}_{I\mathrm{w}}(t), \tag{7.273}$$

which is a hermitian operator, up to a factor i (the direct term in (7.241) does not contribute to a decay process). But then (7.272) becomes

$$\langle\hat{\mathcal{O}}\rangle=\langle\mathrm{i}|\hat{S}_B\hat{\mathcal{O}}\hat{S}_B|\mathrm{i}\rangle=\langle\mathrm{i}_T|\hat{S}_B\hat{\mathcal{O}}_T\hat{S}_B|\mathrm{i}_T\rangle. \tag{7.274}$$

If the initial particle is spinless, then

$$|\mathrm{i}_T\rangle=\eta_T|\mathrm{i}\rangle,\qquad|\eta_T|=1. \tag{7.275}$$

Together with (7.268), this implies

$$\langle \hat{\mathcal{O}} \rangle = 0. \tag{7.276}$$

Thus in a weak decay process, the expectation value of an observable which changes sign under time reversal vanishes. Note that this result is independent of the phase η_T of the decaying particle.

Without the weakness assumption, the exchange of the hermitian conjugation on the scattering operators in (7.272) would have prevented us from any conclusion.

Historically, the invariance under time reversal of weak interactions was apparently assured by the weak decays

$$K^+ \longrightarrow \pi^0 + \bar{\mu}^+ + \nu, \qquad K^- \longrightarrow \pi^0 + \mu^- + \bar{\nu}. \tag{7.277}$$

The outcoming muon was found to have no average polarization orthogonal to the production plane formed by the momenta $\mathbf{p}_\mu$ and $\mathbf{p}_\pi$, i.e., the operator $\hat{\mathcal{O}} = \boldsymbol{\sigma}_\mu \cdot (\hat{\mathbf{p}}_\mu \times \hat{\mathbf{p}}_\pi)$ had no measurable expectation value. Since this operator is odd under time reversal, the vanishing of $\langle \hat{\mathcal{O}} \rangle$ seemed to confirm time-reversal invariance.[7] However, as it turned out later, the breakdown of time-reversal invariance in weak interactions is much too small to be detected by a polarization experiment. There exists a much more sensitive experiment which shows the violation withiut effort: the K^0-$\bar{K}^0$ meson system. This will be discussed later.

7.7.3 Phase of Weak Amplitudes from Time-Reversal Invariance

If a particle decays weakly into two final particles, time-reversal invariance fixes the phase of the decay amplitude, if the final-state interaction is purely elastic, i.e., if there are no other decay channel caused by the final-state interactions. A weak decay can be treated in lowest-order perturbation theory and has the amplitude

$$t_{ba} = \langle \mathrm{f}(-)|\hat{H}_{\mathrm{w}}|\mathrm{i}(+)\rangle, \tag{7.278}$$

where the labels $(\pm)$ indicate that the states contain the full effect of the initial- and final-state interactions (see Section 7.6). From time-reversal invariance we find

$$\langle \mathrm{f}(-)|\hat{H}_{\mathrm{w}}|\mathrm{i}(+)\rangle = \langle \mathrm{i}_T(-)|\hat{H}_{\mathrm{w}}|\mathrm{f}_T(+)\rangle = \langle \mathrm{f}_T(+)|\hat{H}_{\mathrm{w}}|\mathrm{i}_T(-)\rangle^*. \tag{7.279}$$

If we choose the phasefactors η_T of initial and final particles to be unity [see (3.218)], we obtain

$$\langle \mathrm{f}(-)|\hat{H}_{\mathrm{w}}|\mathrm{i}(+)\rangle = \langle \mathrm{f}_T(+)|\hat{H}_{\mathrm{w}}|\mathrm{i}_T(-)\rangle^*. \tag{7.280}$$

The initial state is a stationary single particles state if the weak interactions are ignored. Hence

$$|\mathrm{i}(+)\rangle \approx |\mathrm{i}(-)\rangle. \tag{7.281}$$

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[7] This possibility of testing time-reversal invariance of weak interactions was pointed out by J.J. Sakurai, Phys. Rev. **109**, 980 (1958). See also M. Gell-Mann and A.H. Rosenfeld, Ann. Rev. Nucl. Sci. **7**, 407 (1957), Appendix A.

We now rotate the matrix element on the right-hand side by 180 degrees in the center of mass frame, we reverses momentum and spin directions and bring the time-reversed state back to the original form. Thus we obtain

$$\langle b(-)|\hat{H}_{\rm w}|a(+)\rangle = \langle b(+)|\hat{H}_{\rm w}|a(+)\rangle^*. \tag{7.282}$$

The amplitudes with + and minus interchanged differ by a pure phase factor which is the scattering amplitude for the two-particle scattering in final state:

$$\langle b(-)|\hat{H}_{\rm w}|a(+)\rangle = e^{2i\delta}\langle b(+)|\hat{H}_{\rm w}|a_T(-)\rangle, \tag{7.283}$$

The pure-phase anture is a consequence of the assumption of elasticity. Together with (7.282), this fixes the phases

$$\langle b(\mp)|\hat{H}_{\rm w}|a(+)\rangle = \text{const}\,. \times e^{i\delta}. \tag{7.284}$$

This equation has many applications in phenomenologicl analyses.[8]

Notes and References

For more details on scattering theory see
M.L. Goldberger and K.N. Watson, *Collision Theory*, John Wiley and sons, New York 1964.
S. Schweber, *Relativistic Quantum Fields*, Harper and Row, N.Y., N.Y., 1961

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[8] G. Takeda, Phys. Rev. *101*, 1547 (1956).

8

Quantum Field Theoretic Perturbation Theory

In this chapter we would like to develop a method for calculating the physical consequences of a small interaction in a nearly free quantum field theory.

8.1 The Interacting n-Point Function

We consider an interacting quantum field theory with a time-independent Hamiltonian. All physical informations on the theory are carried by the n-point functions

$$G^{(n)}(x_1,\dots,x_n) \;=\; {}_H\langle 0|T\phi_H(x_1)\phi_H(x_2)\cdots\phi_H(x_n)|0\rangle_H. \tag{8.1}$$

Here $|0\rangle_H$ is the Heisenberg ground state of the interaction system, i.e., the lowest steady eigenstate of the full Schrödinger Hamiltonian:

$$H|0\rangle_H = E|0\rangle_H. \tag{8.2}$$

The fields $\phi_H(x)$ are the fully interacting time-dependent Heisenberg fields, i.e., they satisfy

$$\phi_H(\mathbf{x},t) = e^{-iHt}\phi_S(\mathbf{x})e^{iHt} \tag{8.3}$$

where

$$H = H_0 + V \tag{8.4}$$

is the full Hamiltonian of the scalar field. Note that the field on the right-hand side of Eq. (8.3) has the time argument $t=0$ and is therefore the same in any picture $\phi_I(\mathbf{x},0) = \phi_H(\mathbf{x},0) = \phi(\mathbf{x},0)$ so that we shall also write

$$\phi_H(\mathbf{x},t) = e^{-iHt}\phi(\mathbf{x},0)e^{iHt}. \tag{8.5}$$

We now express $\phi_H(x)$ in terms of the field $\phi_I(x)$ of the interaction picture and rewrite

$$\begin{aligned} G^{(n)}(x_1,\dots,x_n) \;=\; & {}_H\langle 0|T\left[U_I(0,t_1)\phi_I(x_1)U_I(t_1,t_2)\phi_I(x_2)\cdots\right.\\ & \left.\cdots U_I(t_{n-1},t_n)\phi_I(x_n)U_I(t_n,0)\right]|0\rangle_H \end{aligned} \tag{8.6}$$

where we have used the properties of the time displacement operator

$$\begin{aligned} U_I^{-1}(t,0) &= U_I(0,t), \\ U_I(t_1,t_2) &= U_I(t_1,0)U_I^{-1}(0,t_2). \end{aligned} \tag{8.7}$$

We shall now assume that the state $|0\rangle_H$ is a non-degenerate eigenstate of the full Hamiltonian. Then we can make use of the switching-on procedure of the interaction, and the vacuum state must develop for $t \to -\infty$ towards the vacuum of the free field Hamiltonian H_0. According to the Gell-Mann-Low formula we may write,

$$\begin{aligned} |0\rangle_H &= \frac{U_I(0,-\infty)\,|0\rangle}{\langle 0|U_I(0,\infty)\,|0\rangle}, \\ {}_H\langle 0| &= \frac{\langle 0|U_I(\infty,0)}{\langle 0|U_I(\infty,0)\,|0\rangle}, \end{aligned} \tag{8.8}$$

where $|0\rangle$ is the free-particle vacuum and the presence of the switching parameter η and its limit $\eta \to 0$ at the end are tacitly assumed. Then formula (8.6) becomes

$$\begin{aligned} G^{(n)}(x_1,\dots,x_n) &= \langle 0|U_I(\infty,0)\,T\Big(U_I(0,t_1)\,\phi_I(x_1)U_I(t_1,t_2)\,\phi_I(x_2)\cdots \\ &\qquad \cdots U_I(t_{n-1},t_n)\phi_I(x_n)U_I(t_n,0)\Big)\,U_I(0,-\infty)\,|0\rangle \\ &\times\ 1/\langle 0|U_I(\infty,0)\,|0\rangle\langle 0|U_I(0,-\infty)\,|0\rangle. \end{aligned} \tag{8.9}$$

The product in the denominator can be combined to a single expression using the relation (??):

$$\langle 0|U_I(\infty,0)\,|0\rangle\langle 0|U_I(0,-\infty)\,|0\rangle = \langle 0|U_I(\infty,-\infty)\,|0\rangle = \langle 0|S|0\rangle. \tag{8.10}$$

The numerator consists of the S matrix operator $U_I(\infty,-\infty)$ time-sliced into $n+1$ pieces at $t_1,\dots,t_n$, with $\phi(x_i)$, $i=1,\dots,n$, inserted successively. It is gratifying to observe that due to the definition of the time-ordering operator, the expression can be written in the much more compact fashion

$$T\Big(S\,\phi_I(x_1)\phi_I(x_2)\cdots\phi_I(x_n)\Big), \tag{8.11}$$

so that we arrive at the simple formula

$$\begin{aligned} G^{(n)}(x_1,\dots,x_n) &= \langle 0|T\Big(S\,\phi_I(x_1)\cdots\phi_I(x_n)\Big)|0\rangle/\langle 0|S|0\rangle \qquad (8.12) \\ &= \frac{\langle 0|Te^{-i\int_{-\infty}^{\infty}dt\,V_I(t)}\phi_I(x_1)\cdots\phi_I(x_n)|0\rangle}{\langle 0|e^{-i\int_{-\infty}^{\infty}dtV_I(t)}|0\rangle}. \end{aligned}$$

The fields $\phi_I(x)$ are now expressed as follows: by

$$\begin{aligned} \phi_I(\mathbf{x},t) &= e^{iH_0t}\phi_S(\mathbf{x})e^{-iH_0t} \\ &= e^{iH_0t}\phi(\mathbf{x},0)\,e^{-iH_0t}. \end{aligned} \tag{8.13}$$

This implies that the field $\phi(\mathbf{x},t)$ changes in time in the same way as the Heisenberg field $\phi_H(\mathbf{x},t)$ of the free Hamiltonian H_0 would do with the initial condition $\phi_H(\mathbf{x},0)=\phi(\mathbf{x},0)$. This observation will be the key to the evaluation of the n-point functions.

What is the interaction picture of the interaction V_I itself? We assumed V to be an arbitrary spatial functional of ϕ_S,

$$V=V\left[\phi_S(\mathbf{x})\right]. \tag{8.14}$$

But then we may use (8.13) to calculate

$$V_I(t)=V\left[\phi_I(\mathbf{x},t)\right]. \tag{8.15}$$

Thus the potential $V_I(t)$ in the interaction picture is simply the Schrödinger interaction V with the fields $\phi_S(\mathbf{x})$ replaced by $\phi_I(\mathbf{x},t)$ which develop from $\phi(\mathbf{x},0)$ via the free field equations of motion.

The state $|0\rangle$ is the ground state of the free Hamiltonian H_0, i.e., the vacuum state arising in the free-field quantization of Chapters 3 and 5. If we drop the indices I, we can state the interaction n-particle Green function as

$$G^{(n)}(x_1,\dots,x_n) = \frac{\langle 0|Te^{-i\int_{-\infty}^{\infty}dtV[\phi(\mathbf{x},t)]}\phi(x_1)\cdots\phi(x_n)|0\rangle}{\langle 0|Te^{-i\int_{-\infty}^{\infty}dtV[\phi(\mathbf{x},t)]}|0\rangle}, \tag{8.16}$$

where $\phi(\mathbf{x},t)$ is the free field and $|0\rangle$ the vacuum associated with it.

Note that the functional brackets only hold for the spatial variable $\mathbf{x}$. All fields in $V[\phi(\mathbf{x},t)]$ have the same time argument. In a local quantum filed theory, the functional is a psatial integral over a density

$$e^{-i\int_{-\infty}^{\infty}dt\,V[\phi(\mathbf{x},t)]}e^{-i\int_{-\infty}^{\infty}dt\int d^3x\,v(\phi(\mathbf{x},t))}. \tag{8.17}$$

8.2 Perturbation Expansion for Green Functions

In general, it is very hard to evaluate expressions like (8.16). If the interaction term V_I is very small, however, it is suggestive to perform a power series expansion and write

$$\begin{aligned} e^{-i\int_{-\infty}^{\infty}dtV[\phi(\mathbf{x},t)]} &= 1-i\int_{-\infty}^{\infty}dtV\left[\phi(\mathbf{x},t)\right] \\ &+ \frac{(-i)^2}{2!}\int_{-\infty}^{\infty}dt_1dt_2T\left(V\left[\phi(\mathbf{x}_1,t_1)\right]V\left[\phi(\mathbf{x}_2,t_2)\right]\right)+\dots\,. \end{aligned} \tag{8.18}$$

In this way, we are confronted in (8.16) with the vacuum expectation value of many free fields $\phi(x)$ of which n are from the original product $\phi(x_1)\cdots\phi(x_n)$, the others from the interaction terms. From Wick's theorem we know that we may reduce the expression to a sum over products of free-particle Green functions $G_0(x-x')$ with all possible pair contractions. The simplest formulation of this theorem was given in terms of the generating functional of all free-particle Green functions [recall (5.761)],

$$Z_0[j] = \langle 0|Te^{i\int d^4x\,\phi(x)j(x)}|0\rangle, \tag{8.19}$$

where the subscript 0 emphasizes now the absence of interactions. This functional can also be used to compactly specify the perturbation expansion. Let us introduce the generating functional also for the interacting case, where the Green functions are expectation values of products of Heisenberg field $\phi_H(x)$ in the full Heisenberg vacuum state,

$$Z_H[j] \equiv {}_H\langle 0|Te^{i\int d^4x\,\phi_H(x)j(x)}|0\rangle_H, \tag{8.20}$$

The functional derivatives of this yield the full n-point functions (8.1). The perturbation expansion derived above can now be phrased compactly in the formula

$$Z_H[j] \equiv Z_D[j]/Z[0], \tag{8.21}$$

where $Z[j]$ is the generating functional in the interaction or Dirac picture:

$$Z[j] \equiv \langle 0|Te^{-i\int_{-\infty}^{\infty} dtV[\phi(x)]+i\int d^4x\,\phi(x)j(x)}|0\rangle. \tag{8.22}$$

The fields and the vacuum state in $Z[j]$ are those of the free field theory. Note that $Z_H[j]$ and $Z[j]$ differ only by an irrelevant constant $Z[0]$ which appears in the denominators of all Green functions (8.16), and which has an important physical meaning to be understood in Section 8.3.1. The main difference bestween them is the prescription of how they are to be evaluated.

As functionals of the sources j, That this expression for the generating functional yields the perturbation expansion for all n-point functions can be verified by functional differentiations with respect to j and comparison of the results with (8.16) and (8.1).

Note that while the generating functional $Z_H[j]$ is normalized to unity for $j \equiv 0$, this is not the case for the auxiliary functional $Z[j]$. Nevertheless, for generating n-point functions, $Z[j]$ is just as useful as the properly normalized $Z_H[j]$ if one only modifies the differentiation rule by the overall factor $Z[0]^{-1}$:

$$G^{(n)}(x_1,\dots,x_n) = \left[\frac{1}{Z[j]}\frac{\delta}{i\delta j(x_1)}\cdots\frac{\delta}{i\delta j(x_n)}Z[j]\right]_{j=0}. \tag{8.23}$$

This is what we shall do from on do so that we can refer to $Z[j]$ as a generating functional. This will also be of advantage when we come to enumerating the different perturbative contributions to each Green function. Indeed, formula (8.23) allows for an immediate even though formal and implicit solution for the interacting generating functional: Since differentiation $\delta/\delta j(x)$ produces a field $\phi(x)$ we may rewrite the interaction $V\,[\phi(x)]$ as $V\,[-i\delta/\delta j(x)]$. Then it is no longer a field operator and may be removed from the vacuum expectation value so that $Z[j]$ becomes

$$Z[j] = e^{-i\int_{-\infty}^{\infty} dtV[-i\delta/\delta j(x)]}Z_0[j]. \tag{8.24}$$

Now $Z_0[j]$ was calculated explicitly in (5.438) from Wick's theorem

$$Z_0[j] = \exp\left\{-\frac{1}{2}\int d^4y_1 d^4y_2 j(y_1)G_0(y_1,y_2)j(y_2)\right\}. \tag{8.25}$$

The perturbation series of all n-point functions are now found by expanding the exponential in (8.24) in powers of V and performing the derivatives with respect to $\delta/\delta j(x)$. These produce precisely all Wick contractions involving the fields in the interaction.

The explicit evaluation is quite difficult for an arbitrary interaction. It is therefore advisable to learn dealing with such expressions by considering simple examples.

8.3 Feynman Rules for ϕ^4-theory

In order to understand the systematics of the perturbation expansion let us focus attention on a very simple field theory with the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 + \frac{g}{4!}\phi^4. \tag{8.26}$$

This is usually referred to as ϕ^4-theory. Her m is the mass of the free particles and g the coupling strength. We shall assume g to be small enough to be able to expand all interacting Green function in a power series in g. It is well-known that the resulting series will be divergent since the coefficients of g^k at large order k will grow like $k!$. Fortunately, however, the limiting behavior of the coefficients is exactly known which has made it possible to develop powerful resummation techniques for extracting reliable results from this series.

The interaction in the Schrödinger picture is

$$V\left[\phi_S(\mathbf{x})\right] = \frac{g}{4!}\int d^3x \phi_S^4(\mathbf{x}). \tag{8.27}$$

In the interaction picture, after substituting $\phi_S(x)$ by the free field $\phi(x)$, the exponent in formulas (8.16), (8.22) becomes

$$e^{-i\int_{-\infty}^{\infty} dt V[\phi_S(\mathbf{x},t)]} = e^{-i\frac{g}{4!}\int d^4x\, \phi^4(x)}. \tag{8.28}$$

In the functional formulation of the perturbation expansion we have to calculate the series

$$\begin{aligned} Z[j] &= e^{-i\frac{g}{4!}\int d^4x(-i\delta/\delta j(x))^4} Z_0[j] \\ &= \left[1 - i\frac{g}{4!}\int d^4x\left(-i\frac{\delta}{\delta j(x)}\right)^4\right. \\ &\quad \left. + \frac{(-i)^2}{2!}\left(\frac{g}{4!}\right)^2 \int d^4x_1 d^4x_2 \left(-i\frac{\delta}{\delta j(x_1)}\right)^2 \left(\frac{-i\delta}{\delta j(x_2)}\right)^2 + \dots\right] \\ &\quad \times e^{-\frac{1}{2}\int d^4y_1 d^4y_2 j(y_1)G_0(y_1,y_2)j(y_2)}. \end{aligned} \tag{8.29}$$

The n-point functions are obtained according to (8.23) by expanding the exponential on the right-hand side in a power series, forming the nth functional derivatives with respect to j, and setting j to zero. The result has to be divided by $Z[0]$ which is also a power series in g. Certainly, n has to be even, otherwise the result vanishes. It we want to calculate $G^{(n)}$ up to a given power in g, say g^k, there are many different contributions. The denominator $Z[0]$ has to be expanded in powers of g and its kth- order contributions come from the $\left(-\frac{1}{2}\int jG_0 j\right)^{2k}/(2k)!$ term in the expansion of the exponential. Here and in most of the following structural formulas we shall omit the integration variables, for brevity. The $k^{\rm th}$-order term has the form

$$Z_k[0]=\left(-i\frac{g}{4!}\right)^k\int\left(-i\frac{\delta}{\delta j_1}\right)^4\cdots\left(-i\frac{\delta}{\delta j_k}\right)^4\frac{1}{(2k)!}\left(-\frac{1}{2}\int jG_0 j\right)^{2k}. \tag{8.30}$$

In the numerator of (8.23), there are contributions of zeroth order in g to $G^{(n)}$ from the $(n/2)^{\rm th}$ term which has the form $\left(-\frac{1}{2}\int jG_0 j\right)^{n/2}$, of first order in g form the $(n/2+2)^{\rm th}$ term $\left(-\frac{1}{2}\int jG_0 j\right)^{n/2+2}$, of second order in g from the $(n/2+4)^{\rm th}$ term $\left(-\frac{1}{2}\int jG_0 j\right)^{n/2+4}$, etc. Forming the 4 derivatives $(\delta/\delta j)^4$ associated with every order in g, as well as the n derivatives for the Green function $G^{(n)}$, the expression to $k^{\rm th}$ order have the structure

$$\begin{aligned}&\left(-i\frac{g}{4!}\right)^k\left(-i\frac{\delta}{\delta j_1}\right)\cdots\left(-i\frac{\delta}{\delta j_n}\right)\\&\qquad\times\int\left(-i\frac{\delta}{\delta j}\right)^4\cdots\left(-i\frac{\delta}{\delta j}\right)^4\frac{1}{(n/2+2k)!}\left(-\frac{1}{2}jG_0 j\right)^{\frac{n}{2}+2k}.\end{aligned} \tag{8.31}$$

The Green functions accurate to order g^k are then obtained by dividing the two power series through each other and expanding the result again up to order g^k.

This all seems to be a horrendous task. It is, however, possible to devise a diagrammatic procedure for keeping track of the different contributions which will show that many simplifications arise. In particular, the division process is really quite trivial due to the fact that $Z[0]$ appears automatically as a factor in the calculation of the numerator of each n-point function.

Actually formula (8.29), even though giving the most explicit answer to the problem, is quite cumbersome when it comes to actual calculations. The derivatives are an efficient analytic way of accounting for the set of all Wick contractions between the field operations. In the calculation of a specific n-point function, however, it is much more advantageous to insert the expansion (8.18) into formula (8.16), separate numerator and denominator by writing

$$G^{(n)}(x_1,\dots,x_n)\equiv\frac{1}{Z[0]}\bar{G}^{(n)}(x_1,\dots,x_n), \tag{8.32}$$

with the unnormalized Green function $\bar{G}^{(n)}(x_1,\dots,x_n)$ having the expansion

$$\bar{G}^{(n)}(x_1,\dots,x_n)\equiv$$

$$= \langle 0|T\Big\{\Big(1 - \frac{ig}{4!}\int d^4z\phi(z) + \frac{1}{2!}\left(\frac{-ig}{4!}\right)^2 \int d^4z_1 d^4z_2 \phi^4(z_1)\phi^4(z_2) + \ldots\Big) \\ \times\phi(x_1)\cdots\phi(x_n)\Big\}|0\rangle, \qquad (8.33)$$

and the denominator $Z[0]$ of (8.32)

$$Z[0] = \langle 0|T\left(1 - \frac{ig}{4!}\int d^4z\phi^4(z) + \frac{1}{2!}\left(\frac{-ig}{4!}\right)^2 \int d^4z_1 d^4z_2 \phi(z_1)\phi(z_2) + \ldots\right)|0\rangle, \qquad (8.34)$$

and to perform the Wick contractions in the two expansion explicitly yielding $\bar{G}_p^{(n)}$ and $Z_p[0]$, respectively.

8.3.1 The Vacuum Graphs

Because of its formal simplicity let us start a more explicit perturbation expansion with the calculation of $Z[0]$. To first-order in the coupling constant g we have to find

$$Z_1[0] = -i\frac{g}{4!}\int d^4z\langle 0|T\left(\phi(z)\phi(z)\phi(z)\phi(z)\right)|0\rangle, \qquad (8.35)$$

where we have written down the four powers of $\phi(z)$ separately see better how to perform all pair contractions. The first field can be contracted with the three others. After this the second field has only one choice. Thus there are $3 \cdot 1$ contractions, all of the form

$$-i\frac{g}{4!}\int d^4z G_0(z,z)G_0(z,z), \qquad (8.36)$$

so that

$$Z_1[0] = -i3\frac{g}{4!}\int d^4z G_0(z,z)G_0(z,z). \qquad (8.37)$$

To order g^2 we have to evaluate

$$\frac{1}{2!}\left(-i\frac{g}{4!}\right)^2 \int d^4z_1 d^4z_2 \\ \times\langle 0|T\left(\phi(z_1)\phi(z_1)\phi(z_1)\phi(z_1)\phi(z_2)\phi(z_2)\phi(z_2)\phi(z_2)\right)|0\rangle. \qquad (8.38)$$

Now there are $7 \cdot 5 \cdot 3 \cdot 1 = 105$ contraction, 3^2 of them with $\phi(z_1)$'s and $\phi(z_2)$'s contracting among each other, for example,

$$\dot{\phi}(z_1)\dot{\phi}(z_1)\ddot{\phi}(z_1)\ddot{\phi}(z_1)|\overset{\cdot}{\ddot{\phi}}(z_2)\overset{\cdot}{\ddot{\phi}}(z_2)\overset{\cdot\cdot}{\ddot{\phi}}(z_2)\overset{\cdot\cdot}{\ddot{\phi}}(z_2). \qquad (8.39)$$

where we have explicitly separated the two interactions by a vertical line. There are further $4 \cdot 3 \cdot 2 = 24$ contractions, where each $\phi(z_1)$ connects with a $\phi(z_2)$, for example,

$$\dot{\phi}(z_1)\ddot{\phi}(z_1)\overset{\cdot}{\ddot{\phi}}(z_1)\overset{\cdot\cdot}{\dot{\phi}}(z_1)|\overset{\cdot\cdot}{\ddot{\phi}}(z_2)\overset{\cdot}{\ddot{\phi}}(z_2)\ddot{\phi}(z_2)\dot{\phi}(z_2), \qquad (8.40)$$

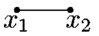
and $6 \cdot 6 \cdot 2 = 72$ of the mixed type, for example,

$$\dot{\phi}(z_1)\dot{\phi}(z_1)\ddot{\phi}(z_1)\dddot{\phi}(z_1)|\dddot{\phi}(z_2)\ddot{\phi}(z_2)\ddddot{\phi}(z_2)\ddddot{\phi}(z_2). \tag{8.41}$$

The factors six counts the six choices of one contraction within each factor ϕ^4 after which there are only two possible interconnections.
The 105 terms obtained in this way correspond to the following integrals

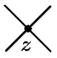
$$\frac{1}{2!}\left(-i\frac{g}{4!}\right)^2\left[9\left(\int d^4z_1G_0(z_1,z_1)^2\right)^2+24\int d^4z_1d^4z_1G_0\left(z_1,z_2\right)^4\right.$$
$$\left.+72\int d^4zd^4zG_0(z_1,z_1)G_0(z_1,z_2)^2G_0\left(z_1,z_2\right)^2G_0(z_2,z_2)\right]. \tag{8.42}$$

It is useful to picture the different contributions by means of so-called *Feynman diagrams*: A line with x_1, x_2 at the ends



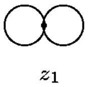
$$= G_0(x_1, x_2) \tag{8.43}$$

represents a free-particle propagator. A vertex with four emerging lines



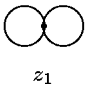
$$= -i\frac{g}{4!} \tag{8.44}$$

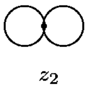
stands for the $\phi^4(z)$ interaction at the point z with the convention to carry a coupling constant $-ig/4!$. The spacetime variables of each vertex have to be integrated over. Then the only diagram to first order is

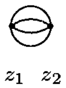
3 

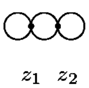
(8.45)

To second order there are three diagrams

9 



+ 24 

+ 72 

. (8.46)

To third order we finds $11 \cdot 9 \cdot 7 \cdot 5 \cdot 3 \cdot 1 = 10395$ terms. The total number rapidly proliferates.

Diagrams of this type consisting only of lines which close back with each other are called *vacuum diagrams*.

When discussing Eq. (5.130) we have noted an important statstical interpretation of the relativistic euclidean propagator $G(x, x')$. It describes the probability for a random walk of any length τ to go from x to x', with a length distribution governed by a Boltzmann-like factor $e^{-\mu\tau}$. The loop expansion of the partition function in terms of vacuum diagrams may therefore be interpreted as a direct picture of the various topologies of random lines in a grand-canonical ensemble of lines of any length. For this reason, relativistic quantum field theories may be used to study such line ensembles, in which case they are called disorder field theories. As mentioned in Chapter 5, such lines appear in many physical systems in the form of vortex lines and defect lines.[1] Details will be discussed in Chapter 19.

8.4 The Two-Point Function

Let us now turn to the numerator in the perturbation expansion for the n-point function (8.29). We shall first study the two-point function. Clearly, to zeroth order there is only the free-particle expression

$$\bar{G}^{(2)}(x_1,x_2) = \langle 0|T\phi(x_1)\phi(x_2)|0\rangle = G_0\,(x_1,x_2) \tag{8.47}$$

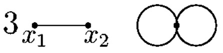
corresponding to the Feynman diagram (8.43). To first order we have to find all contractions of the expression

$$\frac{-ig}{4!}\int d^4z\langle 0|T\phi(z)\phi(z)\phi(z)\phi(z)\phi(z_1)\phi(z_2)|0\rangle. \tag{8.48}$$

There are $5\cdot 3\cdot 1 = 15$ of them. They fall into two classes: 3 diagrams contain contractions only among $\phi(z)$'s multiplied by a contraction of $\phi(x_1)$ with $\phi(x_2)$. Analytically, they correspond to

$$3\left(\frac{-ig}{4!}\right)\int d^4zG_0^2(z,z)G_0\,(x_1,x_2) \tag{8.49}$$

i.e., this expression carries the same factor 3 that was found in the calculation (8.36) of the vacuum diagrams by themselves. The diagrammatic representation consists of a line and the vacuum diagram side by side

3 

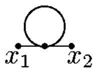
. (8.50)

Such a diagram is called *disconnected*. In general, the analytic expression corresponding to disconnected diagrams is the product of the expressions corresponding to the individual pieces.

The second class of first-order diagrams collects the contractions between $\phi(z)$'s and $\phi(x_1)$ or $\phi(x_2)$. There are 12 of them with the analytic expression

$$12\left(\frac{-ig}{4!}\right)\int d^4zG_0\,(x_1,z)\,G_0\,(z,z)\,G_0\,(z,x_2)\,. \tag{8.51}$$

They are pictured by the connected Feynman diagram



. (8.52)

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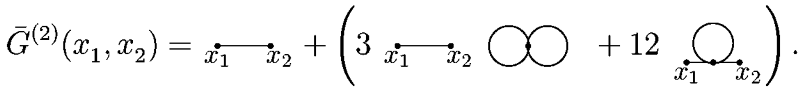
[1] See the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, World Scientific, 1989 (http://www.physik.fu-berlin.de/~kleinert/kleiner_re.html#b1), and H. Kleinert, *Proceedings of a NATO Advanced Study Institute on Formation and Interactions of Topological Defects* at the University of Cambridge, England (cond-mat/9503030).

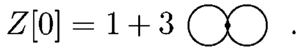
Thus the expansion to first order has the diagrammatic expansion



$\bar{G}^{(2)}(x_1,x_2) =$
x_1
x_2
$+$
3
$+12$

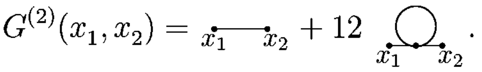
(8.53)

Remembering the expansion of the denominator to this order



(8.54)

we see that the two-particle Green function is to order g given by the free diagram and the diagram in Fig. 8.52.



$G^{(2)}(x_1,x_2) =$
x_1
x_2
$+12$

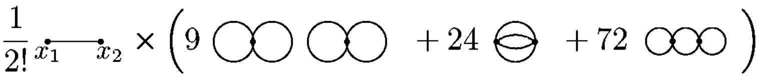
(8.55)

The disconnected pieces involving the vacuum diagram have canceled.

Consider now the second-order contributions. To obtain $\bar{G}$ we have to form all contractions of

$$\frac{1}{2!}\left(\frac{-ig}{4!}\right)^2\int d^4z_1d^4z_2\langle 0|T\phi\,(z_1)\,\phi(z_1)\phi(z_1)\phi(z_1)\phi(z_2)\phi(z_2)\phi(z_2)\phi(z_2)$$
$$\times\phi(x_1)\phi(x_2)|0\rangle. \tag{8.56}$$

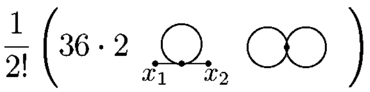
There are $9\cdot7\cdot5\cdot3\cdot1=945$ of them. These decompose into three classes. The first is disconnected and contains the 105 vacuum diagrams multiplied by $G_0(x_1,x_2)$,



$\frac{1}{2!}$
x_1
x_2
$\times$
9
$+24$
$+72$

(8.57)

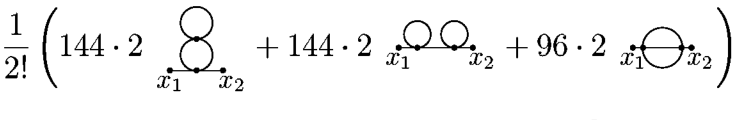
The second consists of mixed contributions in which the first order correction to $\bar{G}$ combined with a first-order vacuum diagram



$\frac{1}{2!}$
$36\cdot2$
x_1
x_2

(8.58)

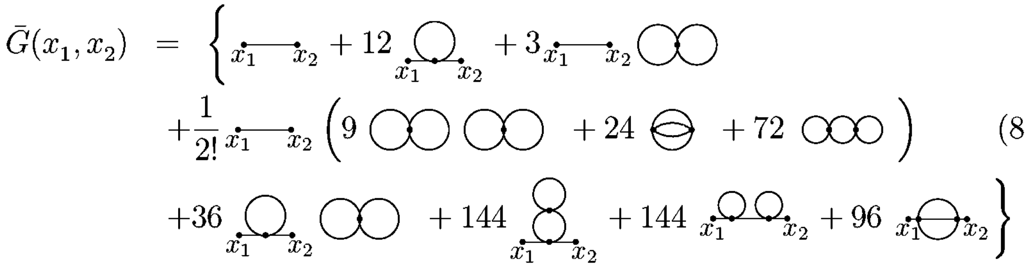
The third contained only the connected diagrams



$\frac{1}{2!}$
$144\cdot2$
x_1
x_2
$+144\cdot2$
$+96\cdot2$

(8.59)

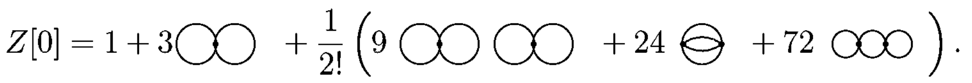
In order to calculate the two-point function up to order g^2 we have to divide



$\bar{G}(x_1,x_2) =$
x_1
x_2
$+12$
$+3$
$+\frac{1}{2!}$
9
$+24$
$+72$
$+36$
$+144$
$+144$
$+96$

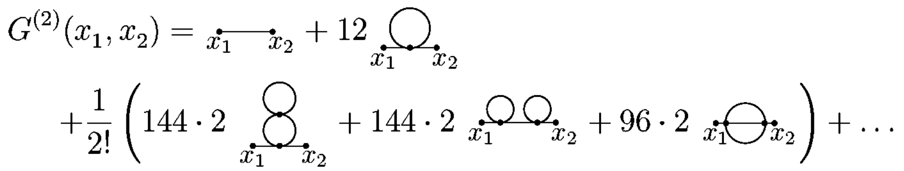
(8.60)

by $Z[0]$ calculated up to the same order which consists of the diagrams


$Z[0] = 1 + 3$
$+ \frac{1}{2!}\Big(9$
$+ 24$
$+ 72$
$\Big).$

(8.61)

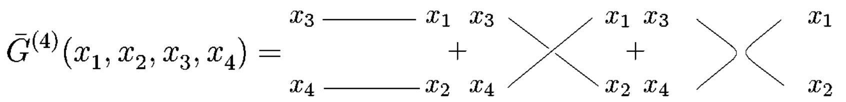
Dividing $\bar{G}$ by $Z[0]$ gives the two-point function


$G^{(2)}(x_1, x_2) =$
x_1
x_2
$+ 12$
x_1
x_2
$+ \frac{1}{2!}\Big(144 \cdot 2$
x_1
x_2
$+ 144 \cdot 2$
x_1
x_2
$+ 96 \cdot 2$
x_1
x_2
$\Big) + \ldots$

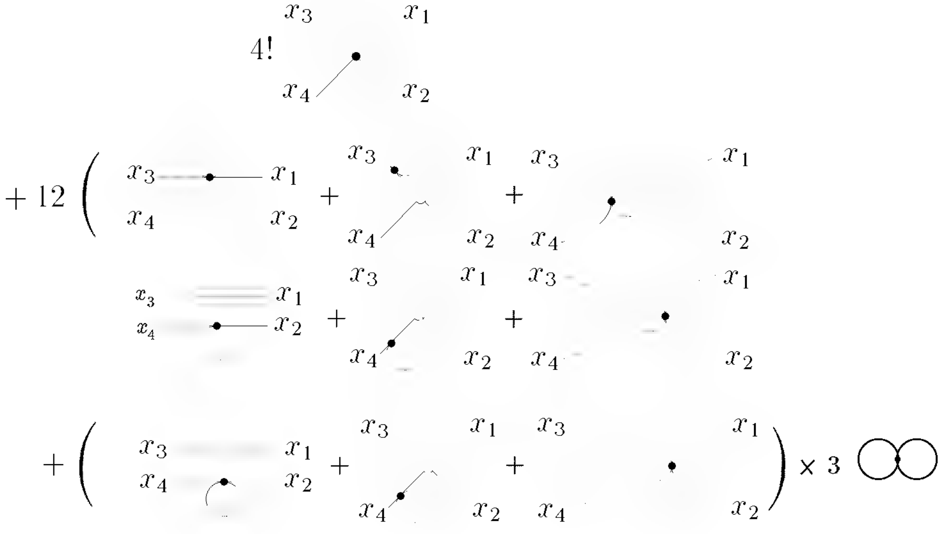
(8.62)

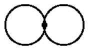
8.5 The Four-Point Function

Let us now study the four-point function. To zeroth order, the numerator has the following trivial contributions

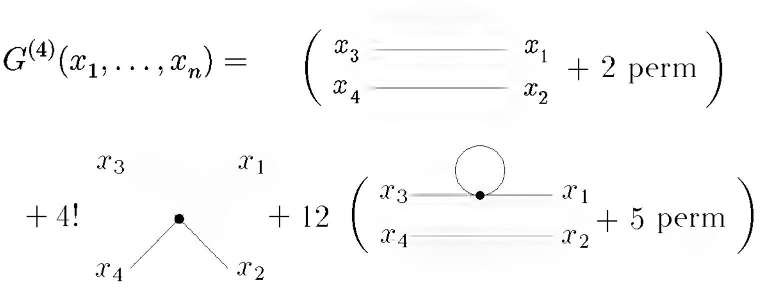

$\bar{G}^{(4)}(x_1, x_2, x_3, x_4) =$
x_3
x_4
x_1
x_2
$+$
x_3
x_4
x_1
x_2
$+$
x_3
x_4
x_1
x_2

To first order there are the diagrams

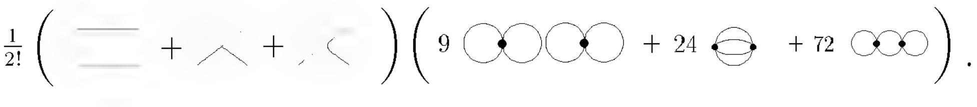

4!
x_3
x_1
x_4
x_2
$+ 12$
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
$+$
x_3
x_1
x_4
x_2
$\times 3$

We observe again the appearance of a factor $1 + 3$  containing the first-order vacuum diagram, which is canceled when forming the quotient (8.32). Thus $G^{(4)}$ can be written to this order as

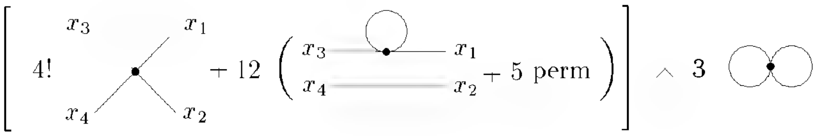
$G^{(4)}(x_1,\dots,x_n) =$


x_3
x_1
x_4
x_2
+ 2 perm
+ 4!
x_3
x_1
x_4
x_2
+ 12
x_3
x_1
x_4
x_2
+ 5 perm

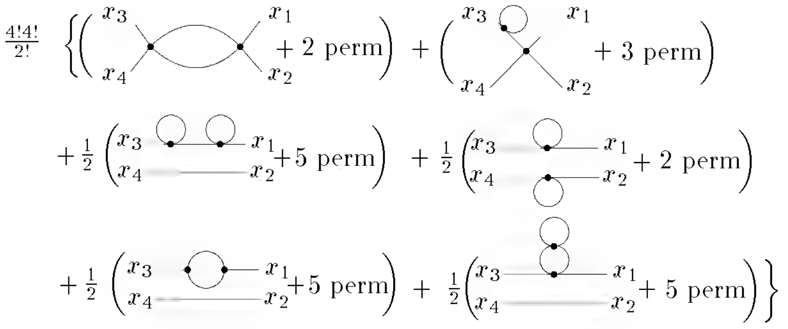
To second order there are $11 \cdot 9 \cdot 7 \cdot 5 \cdot 3 \cdot 1 = 10395$ diagrams in $\bar{G}^{(4)}(x_1,x_2,x_3,x_4)$. They consist of 105 vacuum diagrams of second order multiplied with the zeroth-order diagram in $\bar{G}^{(4)}(x_1,x_2,x_3,x_4)$:


$\frac{1}{2!}$
+
+
9
+ 24
+ 72
.

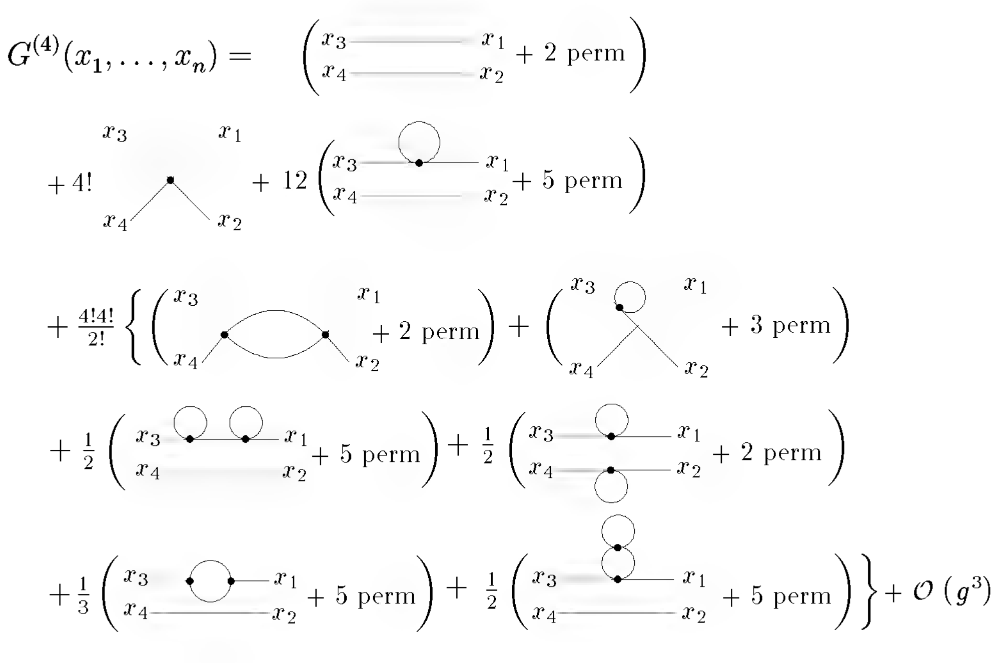
Then there are those in which the vacuum diagrams appear in first order


x_3
x_1
4!
x_4
x_2
+ 12
x_3
x_1
x_4
x_2
+ 5 perm
× 3

And finally there are 9504 terms without vacuum contributions


$\frac{4!4!}{2!}$
x_3
x_1
x_4
x_2
+ 2 perm
+
x_3
x_1
x_4
x_2
+ 3 perm
$+\frac{1}{2}$
x_3
x_1
x_4
x_2
+5 perm
$+\frac{1}{2}$
x_3
x_1
x_4
x_2
+ 2 perm
$+\frac{1}{2}$
x_3
x_1
x_4
x_2
+5 perm
$+\frac{1}{2}$
x_3
x_1
x_4
x_2
+ 5 perm

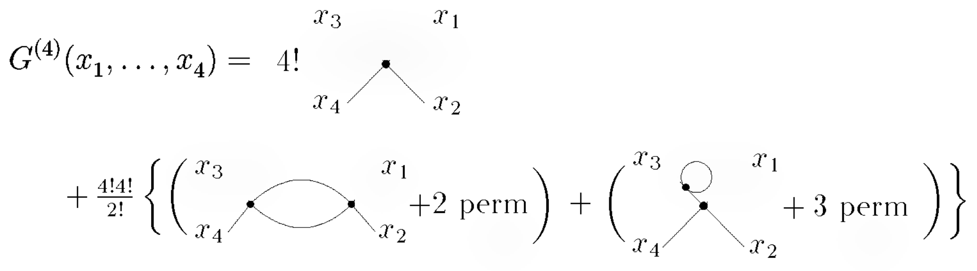
If the vacuum diagrams are divided out we remain with



(8.63)

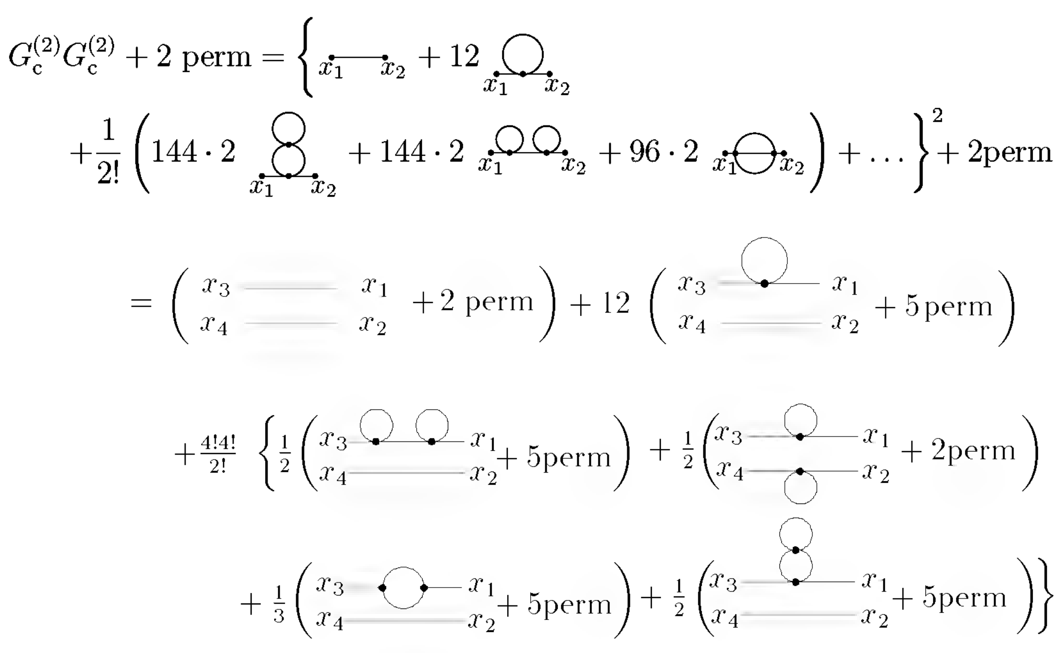
8.6 Connected Green Function

Faced with the rapid proliferation of diagrams for increasing order in the coupling constant, there is need to economize the calculation procedure. The cancellation of all disconnected pieces involving vacuum diagrams was a great simplification. But the remaining diagrams are still many, even at low order in perturbation theory. Fortunately, not all of these diagrams really require a separate calculation. First of all, there are many diagrams which consist of disconnected pieces, each of which already occurs in the expansion (8.62) of the two-point function. since the corresponding amplitude factorizes into the product of the individual expressions, each of these diagrams being really known from the calculation of $G^{(2)}$. Thus, we can save a great deal of labor if we separate the connected diagrams in $G^{(4)}$ and consider them separately. They are called the connected four-point function and denoted by $G_c^{(4)}(x_1,x_2,x_3,x_4)$. Their low-order expansion is simply



We only have to learn how to recover the full Green function from the connected one and the omitted diagrams which are all known from $G^{(2)}$. In the example it can easily be verified that these omitted parts are simply the product of two propagators

$G^{(2)}$ together with the three perturbative corrections on of the external legs



We shall see later that this is a completely general law (if the system is in the so-called *normal phase* as opposed to the *condensed phase* to be studied separately in Chapter 12), i.e., the connectedness structure is

$$G^{(4)}(x_1,\dots,x_n) = G_c^{(4)}(x_1,\dots,x_n) + \left[G_c^{(2)}(x_1,x_2)\,G_c^{(2)}(x_3,x_n) + 2\text{ perm}\right] \tag{8.64}$$

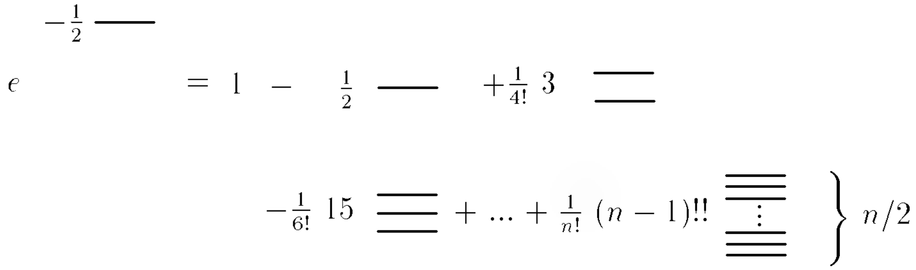
Note that the expansion (8.62) of $G^{(2)}$ is connected. This is a general feature of the normal phase of the theory.

For the higher Green functions we expect more elaborate connectedness relations than (8.64) and an even more drastic reduction of labor using these relations when calculating all diagrams. The question arises as to the general composition law of n-point functions from connected subunits.

To gain a first idea what this law could be, consider the free theory. Its generating functional is [see (5.438)]

$$Z_0[j] = \exp\left\{-\frac{1}{2}\int d^4x\,d^4y\,j(x)G_0(x,y)j(y)\right\}. \tag{8.65}$$

If expanded in powers of j, it gives the sum of all n-point functions of the free theory. In accordance with Wick's theorem all these free n-point functions are disconnected and consist of sums of products of free Green function G_0 which itself is the only connected diagram of the theory. The important point is that the exponential tells us in which way the connected diagrams G_0 can be combined such as to form all diagrams. This may best be visualized diagramically by expanding (8.65) in the form



The numbers after $1/n!$ in the second line show how many combinations of $n/2$ powers of G_0 occur in Wick's expansion. To obtain these numbers we have rewritten the $(n/2)$th coefficient $\frac{1}{(n/2)!}(1/2)^{n/2}$ as $\frac{1}{n!}(n-1)!!$. This establishes contact with the previous counting rules: The denominator $n!$ is factorized out since it is canceled when going to the n-point function (which involves n differentiations $\delta/\delta j$). What is left are $(n-1)!!$ diagrams which is, of course, precisely the result found earlier when counting the diagrams directly. What we have learned from this free-field theory consideration is a simple mnemonic rule for the reconstruction and proper counting of *all* n-point functions given only the connected ones (of which there is only one in this case). We merely have to expand diagramically the exponential $\exp\{-\frac{1}{2}$ ●—● $\}$ and read off all diagrams with n crosses behind the factor $1/n!$. In this way, the exponential of the connected diagram yields all diagrams.

Does this simple statement hold also in the interacting case? Here the generating functional is given by

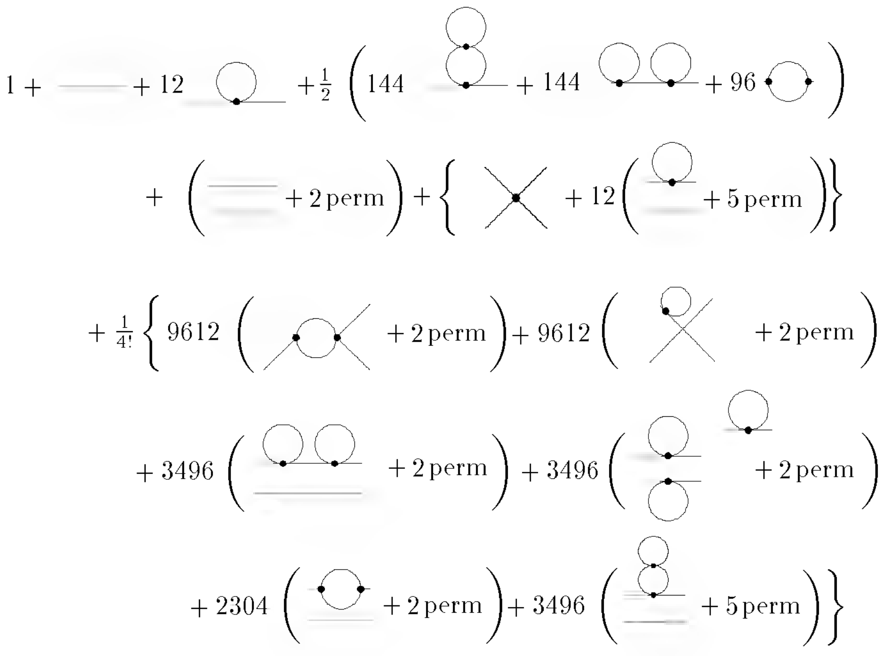
$$Z_0[j] = \exp\left\{i\int d^4x\,\mathcal{L}_{\rm int}\left(\frac{\delta}{i\delta j}\right)\right\}\exp\left\{-\frac{1}{2}\int d^4x\,d^4y\,j(x)G_0(x,y)j(y)\right\}. \quad (8.66)$$

The interactions also enter exponentially. It is therefore suggestive that also here the sum of all Green functions can be obtained by exponentiating all connected ones. The proof will be given later after having developed more powerful formal techniques. Let us state here only the result which may be written as a relation

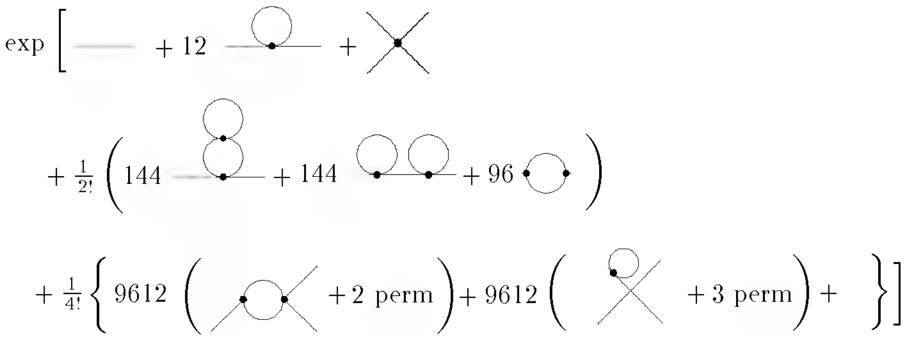
$$1 + \sum_{n=0,k=0}^{\infty}\frac{1}{n!k!}G_k^{(n)} = \exp\left\{\sum_{n=0,k=1}^{\infty}\frac{1}{n!k!}G_{ck}^{(n)}\right\} \quad (8.67)$$

where $G_k^{(n)}$ are all and $G_{ck}^{(n)}$ all connected diagrams in kth-order perturbation theory and the equality holds separately for each number of external lines.

Let us illustrate the statement (8.67) for the previously calculated diagrams for $n = 2$ and $n = 4$. The left-hand side of relation (8.67) looks as follows

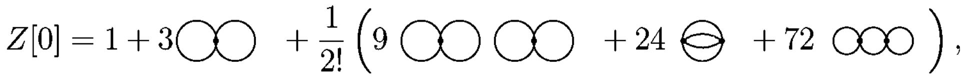

1 +
+ 12
+ 1/2
144
+ 144
+ 96
+
+ 2 perm
+
+ 12
+ 5 perm
+ 1/4!
9612
+ 2 perm
+ 9612
+ 2 perm
+ 3496
+ 2 perm
+ 3496
+ 2 perm
+ 2304
+ 2 perm
+ 3496
+ 5 perm

The right-hand side has the form


exp
+ 12
+
+ 1/2!
144
+ 144
+ 96
+ 1/4!
9612
+ 2 perm
+ 9612
+ 3 perm
+

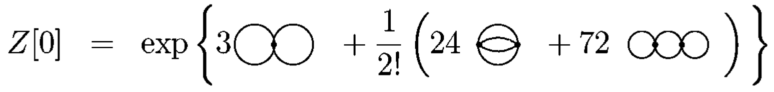
Indeed, by multiplying out the square in the last line we recover the correct sum of disconnected diagrams of the four-point function.

Also the vacuum diagrams satisfy the law of exponentiation: Up to the second order we have for all disconnected pieces


Z[0] = 1 + 3
+ 1/2!
9
+ 24
+ 72

(8.68)

and this can be obtained as an exponential of the connected vacuum diagrams


Z[0] = exp
3
+ 1/2!
24
+ 72

$$\equiv \exp\{W[0]\}. \tag{8.69}$$

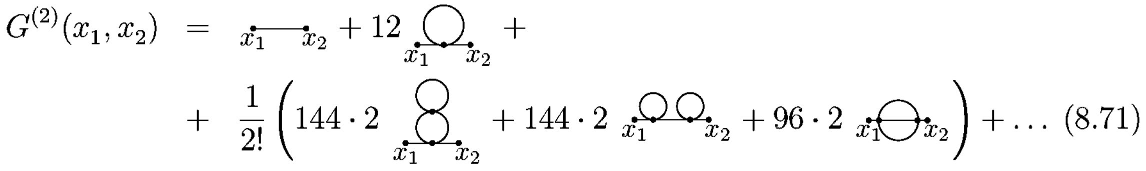
This is equation (8.67) for $n = 0$:

$$1+\sum_{k=0}^{\infty}\frac{1}{k!}G_k^{(0)}=\exp\left[\sum_{k=1}^{\infty}\frac{1}{k!}G_{ck}^{(0)}\right] \tag{8.70}$$

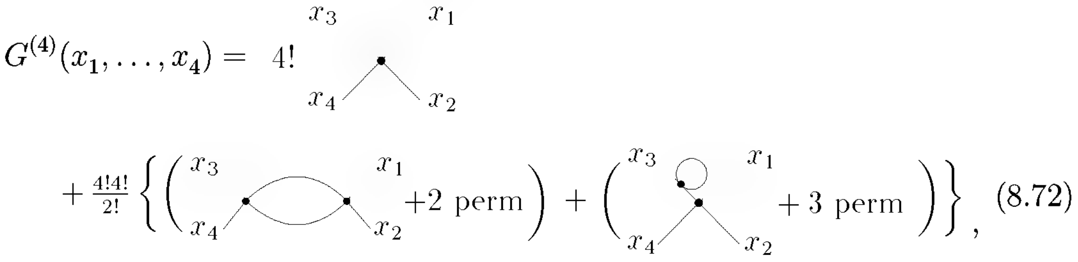
where $G_k^{(0)}$ collect all vacuum diagrams and $G_{ck}^{(0)}$ all connected ones in kth-order perturbation theory. This exponential relation will be of great help when it comes to calculating physical amplitudes and cross sections.

8.6.1 One-Particle Irreducible Graphs

The decomposition into connected diagrams does not yet exhaust the possibilities of reducing calculational labor. If we inspect the connected diagrams for two and four-point functions

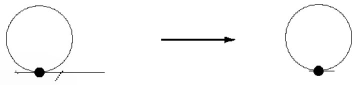


and



we discover that some of the diagrams contain a portion of others calculated at a lower order of perturbation theory in the same connected two-point functions $G_{\rm c}^{(2)}$ or $G_{\rm c}^{(4)}$. An example is the fourth diagram in $G_{\rm c}^{(2)}$. which is a simple repetition of the second one. Similarly, the second diagram in $G_{\rm c}^{(4)}$ is the composition of the first in $G_{\rm c}^{(4)}$ with the second in $G_{\rm c}^{(2)}$. It would be useful to find the rule according to which lower subdiagrams of $G_{\rm c}^{(2)}, G_{\rm c}^{(4)}$ reappear in higher ones of $G_{\rm c}^{(2)}$ and $G_{\rm c}^{(4)}$.

As far as $G_{\rm c}^{(2)}$ is concerned, this rule turns out to be really simple: Let us characterize the repetition of a former subdiagram of $G_{\rm c}^{(2)}$ topologically by noting that the diagram falls into two pieces by cutting one internal line. Such diagrams are called *one-particle reducible* (OPR); otherwise irreducible (OPI). Then the full connected two-point function $G_{\rm c}^{(2)}$ may be composed from all OPI subdiagrams as follows: Consider the set of all OPI diagrams to the two-point function. They all carry a free Green function $G_0^{(2)}$ at the end of each leg which describes propagation of the particle up to the first interaction vertex. Cutting off these last Green functions amounts diagramically to amputating the two legs of the diagram. The lowest order correction to the two-point function is amputated as follows:



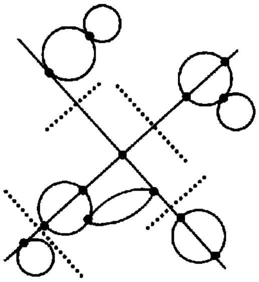
The two short little trunks indicate the places of amputation. Let $-i\Sigma$ be the sum of all these *amputated* OPI two-point functions. Then the geometric series

$$G_{\mathrm{c}}^{(2)} = \frac{1}{G_0^{-1} + \Sigma} = G_0 + G_0(-i\Sigma)G_0 + G_0(-i\Sigma)G_0 + \dots \tag{8.73}$$

gives precisely the connected two-point function $G_{\mathrm{c}}^{(2)}$. Thus the one-particle reducibility in the two-point function exhausts itself in a simple geometric series type of repetition of the irreducible pieces, each term in the string having the same factor. Also this result will be proved later in Chapter when studying the general formal properties of perturbation theory.

The sum of all OPI connected two-point functions $-i\Sigma$ is usually referred to as self-energy.

Consider now the four-point function $G_{\mathrm{c}}^{(4)}$. Here we recognize that any ornamentation of external legs can be taken care of by replacing this leg by the interacting two-point function. Thus we decide to introduce the concept of an arbitrary one-particle irreducible amputated Green function shortly called the *vertex function* $\Gamma^{(n)}(x_1, \dots, x_n)$. For any connected n-point function, cut all simple lines such that the diagrams decompose. What remains are parts with two, four, or more trunks sticking out. The first set consists of the OPI self-energy diagrams discussed before. The others are called three-, four- etc. point vertex parts $\Gamma^{(n)}$, $n = 3, 4, \dots$. For example,

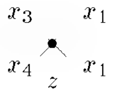


can be cut into four proper self-energy diagrams and one four-point vertex part. The sum of all composite diagrams obtained in this way is the n-point vertex function denoted by . The important reconstruction principle for all diagrams can now be states as follows: The set of all connected diagrams in a four-point function is obtained by connecting all vertex functions in the four-point vertex function $G_{\rm c}^{(4)}$ with the full connected Green function $G_{\rm c}^{(2)}$ at each truncated leg. Analytically, this amounts to the formula (valid in normal systems)

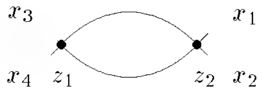
$$G_{\rm c}^{(4)}(x_1,\ldots,x_4)=\int d^4x_1'\,d^4x_2'\,d^4x_3'\,d^4x_4'\;G_{\rm c}^{(2)}(x_1,x_1')\cdots G_{\rm c}^{(2)}(x_4,x_4')\,\Gamma^{(4)}(x_1',\ldots,x_4') \tag{8.74}$$

For the Green function $G_{\rm c}^{(4)}$ as far as it has been calculated in (8.72) we see that it can indeed be decomposed in this way with the vertex function, up to order g^2,

$$i\Gamma_c^{(4)}(x_1,\ldots,x_n) = 4!$$



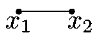
$$+\ \frac{1}{2!}4!^2\left(\right.$$



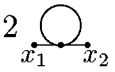
$$\left.+\ 2\ \text{perm}\right) \tag{8.75}$$

and

$$G^{(2)}(x_1,x_2) \ =$$

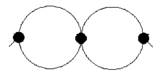


$$+\ 12 \tag{8.76}$$



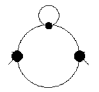
This decomposition of Green functions in terms of vertex functions shows its particular strength when going to higher orders in perturbation theory. Then the number of diagrams to be calculated is greatly reduced. For example, the third-order contribution to the vertex function $i\Gamma_c^{(4)}(x_1,x_2,x_3,x_4)$ are

$$i\Gamma_c^{(4)}(x_1,x_2,x_3,x_4) \ = \ 144\ \left(\right.$$



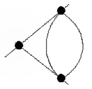
$$\left.+2\ \text{perm}\right)$$

$$+\ 288\ \left(\right.$$



$$\left.+2\ \text{perm}\right)$$

$$+\ 144\ \left(\right.$$



$$\left.+5\ \text{perm}\right) \tag{8.77}$$

We leave it up to the reader to compare this with the diagrams in the connected four-point function $G_{\rm c}^{(4)}$ up to g^3.

For theories more general than ϕ^4 the composition law is more involved and will be discussed in Chapter 6.

8.6.2 Momentum Space Version of Diagrams

The spacetime formulation of Feynman rules will be inconvenient when it comes to an explicit evaluation of diagrams. It will be of great advantage to exploit the translational invariance of the theory by going to momentum space. The free Green function G_0 has the very simple Fourier transform

$$
\begin{aligned}
G_0(q_1,q_2) &\equiv \int d^4x_1 d^4x_2 e^{i(q_1x_1+q_2x_2)} G_0(x_1,x_2) \\
&= \int d^4x_1 d^4x_2 e^{i(q_1x_1+q_2x_2)} \int \frac{d^4}{(2\pi)^4} e^{-iq(x_1-x_2)} \frac{i}{q^2-m^2} \\
&= (2\pi)^4 \delta^{(4)}\left(q_1+q_2\right) G_0(q_1) \qquad (8.78)
\end{aligned}
$$

is the propagator in momentum space. There is an overall $(2\pi)^4\,\delta^{(4)}$-function which ensures the conservation of four momenta. This is a consequence of the translational invariance of $G_0\left(x_1,x_2\right) = G_0\left(x_1-x_2\right)$. The same factor appears in the Fourier transform of all interacting n-point functions since $G^{(n)}\left(x_1,\dots,x_1\right)$ depends only on the differences between the coordinates

$$
G^{(n)}(x_1,\dots,x_n) = G^{(n)}(x_1-x_n, x_2-x_n,\dots,x_{n-1}-x_n,0) \qquad (8.79)
$$

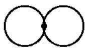
such that we can write

$$
\begin{aligned}
&\int d^4x_1 \dots d^4x_n e^{i\Sigma_{i=1}^n q_i x_i} G^{(n)}(x_1,\dots x_n) \\
&= \int d^4(x_1-x_n)\cdots d^4(x_{n-1}-x_n) e^{i\sum_{i=1}^{n-1} q_i(x_i-x_n)} \left(\int d^4x_n e^{i\Sigma_{i=1}^{\infty} q_i x_n}\right) \\
&\quad G^{(n)}(x_1-x_n, x_2-x_n,\dots,x_{n-1}-x_n,0) \qquad (8.80)
\end{aligned}
$$

Thus we may define the Fourier transform of an n-point function directly with the factor of momentum conservation removed

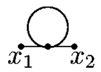
$$
(2\pi)^4\delta^{(4)}\left(q_1+\ldots+q_n\right) G^{(n)}\left(q_1,\dots,q_n\right) \int d^4x_1\cdots d^4x_n \; e^{i\Sigma_{i=1}^n q_i x_i} G^{(n)}\left(x_1,\dots,x_n\right). \qquad (8.81)
$$

Consider now the vacuum diagrams evaluated via the Fourier transforms. To first order we have

3 

$$
= -3i\frac{g}{4!}\int d^4z \;\; G^2(z,z) = -3i\frac{g}{4!}\int d^4z \left[\int \frac{d^4q}{(2\pi)^4}\frac{i}{q^2-m^2}\right]^2 \qquad (8.82)
$$

The integral over z can be defined meaningfully only if the system is enclosed in a finite box of volume V and studied in a finite time interval T. Then the integral $\int d^4z$ gives a factor VT. The integration over the momenta p is still divergent for large p. This is called "ultraviolet divergence". It reflects the singularity of $G_0\left(x_1,x_2\right)$ for $x_1 \longrightarrow x_2$ (a so called short distance singularity). It will be the subject of the next chapter to show how to deal with this type of divergence. For $\bar{G}^{(2)}$ the diagram to first order is

12 

$$
= -12i\frac{g}{4!}\int dz G(x_1,z)G(z,z)G(z,x_2) \qquad (8.83)
$$

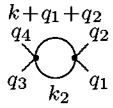
Going to the Fourier transform this gives

$$\int \frac{d^4q}{(2\pi)^4} e^{-iq(x_1-x_2)} \frac{i}{q^2-m^2} \left(\int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2-m^2} \right) \frac{i}{q^2-m^2} \tag{8.84}$$

such that we obtain for the Fourier transformed Green function a contribution

$$\bar{G}^{(2)}(q) = -i\frac{g}{4!}12 \frac{i}{q^2-m^2} \int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2-m^2} \frac{i}{q^2-m^2}. \tag{8.85}$$

As another example take



$$= \left(-\frac{ig}{4!}\right)^2 \int d^4k \frac{i}{k^2-m^2+i\eta} \frac{i}{(k+q_1+q_2)^2-m^2+i\eta} \tag{8.86}$$

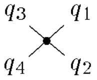
It is easy to see that the following rules hold for the translation of the spacetime diagrams to the analytic expression for the Fourier transformed Green function:

1. With each line associate a momentum label and specify its direction of flow. Then the line corresponds to the Fourier transformed two-point function $G_0(q)$, the free-particle propagator:

   $$\rule{5em}{0.4pt} \quad = \quad G_0(q) = \frac{i}{q^2-m^2} \tag{8.87}$$

   Here the direction of the arrow does not matter since G_0 is symmetric in q.

2. Each vertex

   is associated with an amplitude

   $$-i\frac{g}{4!}(2\pi)^4\delta^{(4)}(q_1+q_2+q_3+q_4) \frac{i}{q_4^2-m^2} \frac{i}{q_3^2-m^2} \frac{i}{q_2^2-m^2} \frac{i}{q_1^2-m^2}$$

   containing a four momentum conservation $(2\pi)^4\,\delta^{(4)}$–function for the incoming momenta. This is a consequence of the integration over z in the interaction.

3. We now distinguish external lines with at least one open and internal lines which connect two vertices with each other. We also call the corresponding momenta q_i external and internal. Then for every internal, lines integrate over all the internal four momentum q_i with the measure $\int d^4q_i/(2\pi)^4$. At the end remove an overall δ-function of energy-momentum conservation.

Obviously, all $(2\pi)^4\delta^{(4)}$-functions associated with the vertices cancels one internal momentum integral $\int d^4p/(2\pi)^4$. Thus in a diagram of nth order with I internal lines, only $I-n$ internal integrations remain. These are referred to as *loop integrals.*

In general, loop integrals there are divergent at large q, in the so-called called the *ultraviolet regime.* We shall learn in the next chapter how to deal with such divergent momentum space integrals.

8.7 Green Functions and Scattering Amplitudes

The Green functions carry all informations contained in the theory. In particular they can be used to extract scattering amplitudes. For definiteness, let us discuss here the simplest and most important case of the elastic scattering among two particles. The free initial state long before the interaction takes place is

$$|\psi_{\rm in}\rangle = a^\dagger_{\mathbf{q}_2} a^\dagger_{\mathbf{q}_1}|0\rangle. \tag{8.88}$$

Long after the interaction the state is given by

$$U_I^\eta(\infty,-\infty)\, a^\dagger_{\mathbf{q}_2} a^\dagger_{\mathbf{q}_1}|0\rangle \tag{8.89}$$

If we analyze this state according to its free-particle content we find the amplitudes

$$\langle 0|a_{\mathbf{q}_4} a_{\mathbf{q}_3} U_I^\eta(\infty,-\infty)\, a^\dagger_{\mathbf{q}_2} a^\dagger_{\mathbf{q}_1}|0\rangle = \langle 0|a_{\mathbf{q}_4} a_{\mathbf{q}_3} S^\eta a_{\mathbf{q}_2} a_{\mathbf{q}_1}|0\rangle \tag{8.90}$$

We shall soon observe that this amplitude has a divergent phase as the switching parameter η tends to zero. This is caused by the same vacuum diagrams as before in the corresponding Green function. In order to obtain a well-defined $\eta \to 0$ -limit we define the 2×2 scattering amplitude as the ratio

$$S(\mathbf{q}_4\mathbf{q}_3|\mathbf{q}_1\mathbf{q}_2) \equiv \frac{S_N(\mathbf{q}_4\mathbf{q}_3|\mathbf{q}_1\mathbf{q}_2)}{Z[0]}, \tag{8.91}$$

with the numerator

$$S_N(\mathbf{q}_4\mathbf{q}_3|\mathbf{q}_1\mathbf{q}_2) \equiv \langle 0|a_{\mathbf{q}_4} a_{\mathbf{q}_3} T e^{-i\int_{-\infty}^{\infty} dt\, V_I(t)} a^\dagger_{\mathbf{q}_2} a^\dagger_{\mathbf{q}_1}|0\rangle \tag{8.92}$$

and the denominator

$$Z[0] \equiv \langle 0|e^{-i\int_{-\infty}^{\infty} dt\, V_I(t)}|0\rangle. \tag{8.93}$$

It is now easy to see how these amplitudes can be extracted from the Green functions calculated in the last section. For this we observe that $a_{\mathbf{q}}, a^\dagger_{\mathbf{q}}$ can be written as

$$a_{\mathbf{q}} = \lim_{x^0\to-\infty} \sqrt{\frac{2q^0}{V}} \int d^3x e^{i(q^0x^0-\mathbf{qx})}\phi(x), \tag{8.94}$$

$$a^\dagger_{\mathbf{q}} = \lim_{x^0\to\infty} \sqrt{\frac{2q^0}{V}} \int d^3x e^{-i(q^0x^0-\mathbf{qx})}\phi(x), \tag{8.95}$$

if q^0 is placed on the mass shell of the particles, i.e., $q^0 = \omega_{\mathbf{q}} = \sqrt{\mathbf{p}^2+M^2}$. The infinite-time limits have the important effect of eliminating the positive or negative frequency contents in $\phi(x)$. Indeed, if we expand the field into creation and annihilation operators we see that the right-hand side of Eq. (8.94) becomes

$$\begin{aligned}&\lim_{x^0\to-\infty} \sqrt{\frac{2q_0}{V}} \int d^3x e^{i(q^0x^0-\mathbf{qx})} \sum_{\mathbf{q}} \frac{1}{\sqrt{2p^0V}} \left(e^{-ipx}a_{\mathbf{p}} + \text{c.c.}\right)\\ &\quad = \lim_{x^0\to-\infty} \sum_{\mathbf{p}} \delta_{\mathbf{p},\mathbf{q}} \left[e^{i(q^0-p^0)x^0} a_{\mathbf{p}} + e^{i(q^0+p^0)x^0} a^\dagger_{\mathbf{p}}\right].\end{aligned} \tag{8.96}$$

The spatial δ-function enforces $\mathbf{q} = \mathbf{p}$ and thus $q^0 = p^0$, so that the right-hand side becomes

$$a_{\mathbf{q}} + \lim_{x^0 \to -\infty} e^{i2q^0x^0} a^\dagger_{\mathbf{q}}. \tag{8.97}$$

In the limit $x^0 \to -\infty$, the second exponential function oscillates infinitely rapidly. Such an oscillating expression can be set equal to zero. The argument why this can be done uses the fact that no physical state is completely sharp in momentum space but contains some, possibly very narrow, distribution function $f(\mathbf{q} - \mathbf{q}')$ in the momenta, and Thus, instead of $a_{\mathbf{q}}$ we really want to consider a state

$$\int \frac{d^3q'}{(2\pi)^3} f(\mathbf{q} - \mathbf{q}') a_{\mathbf{q}'}$$

with $f(\mathbf{q} - \mathbf{q}')$ sharply peaked around $\mathbf{q}$. Then Eq. (8.102) has to be smeared out with such a function, and the second term in (8.97) becomes

$$\lim_{x^0 \to -\infty} \int \frac{d^3q'}{(2\pi)^3} e^{i2q'^0x^0} f(\mathbf{q} - \mathbf{q}') a^\dagger_{\mathbf{q}'} \to 0. \tag{8.98}$$

The vanishing of this in the limit $x^0 \to -\infty$ is a well-known consequence of the Riemann-Lebesgue Lemma. The other equation (8.95) is proved similarly.

We can now make use of formula (8.95), replace the operators $a_{\mathbf{q}}, a^\dagger_{\mathbf{q}}$ by time-ordered fields $\phi(x)$, and obtain for the numerator part of the S matrix elements in Eq. (8.92) the following expression:

$$S_N(\mathbf{q}_4\mathbf{q}_3|\mathbf{q}_2\mathbf{q}_1) = \frac{\sqrt{2^4 q_1^0 q_2^0 q_3^0 q_4^0}}{V^2} \lim_{\substack{x_1^0 > x_2^0 \to \infty \\ x_4^0 < x_3^0 \to -\infty}} e^{i\left[q_4^0x_4^0 - \mathbf{q}_4\mathbf{x}_4 + q_3^0x_3^0 - \mathbf{q}_3\mathbf{x}_3 - q_2^0x_2^0 + \mathbf{q}_2\mathbf{x}_2 - q_1^0x_1^0 + \mathbf{q}_1\mathbf{x}_1\right]}$$
$$\times \langle 0|T\phi(x_4)\phi(x_3)S\phi(x_2)\phi(x_1)|0\rangle. \tag{8.99}$$

The last factor is precisely the four-point function $G^{(4)}(x_4, x_3, x_2, x_1)$.

This formula looks somewhat cumbersome to implement in an actual calculation of the scattering amplitudes and it is useful to simplify it by evaluating the infinite-time limits more explicitly. We observe that the perturbation series for $G^{(n)}(x_n, \ldots, x_1)$ consists of sums of products of free two-point functions G_0 which contain for each spacetime argument $x_1, x_2, \ldots, x_n$ in $G^{(n)}$ a two-point function G_0 whose line ends at that point. Consider, for example, the point x_1, and an associated $G_0(z_1, x_1)$. The operation (8.96) at this point corresponds to taking the limit

$$\sqrt{\frac{2q_1^0}{V}} \lim_{x_1^0 \to -\infty} \int d^3x_1 e^{-i(q_1^0x_1^0 - \mathbf{q}_1\mathbf{x}_1)} \int \frac{d^4q}{(2\pi)^4} e^{-iq(z-x_1)} \frac{i}{q^2 - m^2 + i\eta}. \tag{8.100}$$

The spatial integral over $\mathbf{x}_1$ enforces $\mathbf{q} = \mathbf{q}_1$. The remaining integral over dq^0 can be done via Cauchy's residue theorem. Since $x_1^0 \to -\infty$, the contour of integration may be closed in the lower half of the complex q^0-plane, where it contains only a pole at $q^0 = \omega_{\mathbf{q}_1} = \sqrt{\mathbf{q}_1^2 + m^2} - i\eta$. Thus the integral over q^0 can be done trivially, and we find, that the limit (8.99) has the effect of replacing in the Green functions $G(z, x_1)$ of the incoming external leg as follows:

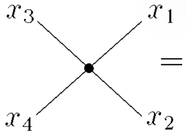
$$G(z, x_1) \longrightarrow \frac{1}{\sqrt{2q_1^0 V}} e^{-iq_1 z}, \tag{8.101}$$

with q_1^0 on the mass shell $q_1^0 = \sqrt{\mathbf{q}_1^2 + m^2}$. The right-hand side is simply the wave function $e^{-iq_1 z}/\sqrt{2q_1^0 V}$ of the incoming particle with the argument z of the nearest vertex in the Feynman diagram.

Similarly, we obtain for an outgoing particle of momentum q_3 the replacement

$$G(x_3, z) \longrightarrow \frac{1}{\sqrt{2q_3^0 V}} e^{iq_3 z} \tag{8.102}$$

As a specific example, consider the simple vertex diagram in (8.72):



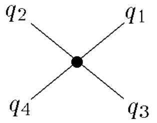
$$= -ig \int d^4z \;\; G(x_4, z) G(x_3, z) G(z, x_2) G(z, x_1). \tag{8.103}$$

Taking the limits (8.99) we obtain

$$\prod_{i=1}^{4} \left(\frac{1}{\sqrt{2Vq_i^0}} \right) (-ig) \int d^4z \;\; e^{i(q_4 z + q_3 z - q_1 z - q_2 z)}$$
$$= -ig \prod_{i=1}^{4} \left(\frac{1}{\sqrt{2Vq_i^0}} \right) (2\pi)^4 \delta^{(4)} \left(q_4 + q_3 - q_2 - q_1 \right). \tag{8.104}$$

Thus, up to a factor $1/\sqrt{2Vq_i^0}$ for each particle, we remain precisely with the vertex contribution in momentum space including the total four-momentum conservation factor.

In momentum space the Feynman diagram (8.103) reads



$$= \quad -ig \frac{i}{q_4^2 - m^2} \frac{i}{q_3^2 - m^2} \frac{i}{q_2^2 - m^2} \frac{i}{q_1^2 - m^2}$$

Thus, by replacing the four external lines by external physical particles of momenta q_i corresponds to dropping the factors

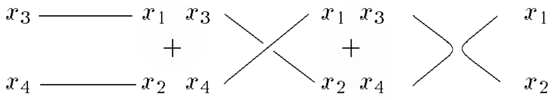
$$\frac{i}{q_i^2 - m^2}$$

and replacing them by

$$\frac{1}{\sqrt{2Vq_i^0}}.$$

This corresponds to the amputation of the Feynman diagram for the four-point function introduced earlier when defining the vertex functions.

How about the disconnected diagrams in (8.63)? Consider first the three diagrams containing two disconnected lines



In each of the diagrams we have to do the operations of the type (8.88). Take the first diagram and consider $G_0\left(x_3, x_1\right)$. It contributes a factor

$$\sqrt{\frac{2q_3^0}{V}}\sqrt{\frac{2q_1^0}{V}} \lim_{\substack{x_3^0\to\infty \\ x_1^0\to-\infty}} \int d^3x_3 d^3x_1 \;\; e^{i\left[q_3^0x_3^0-\mathbf{q}_3\mathbf{x}_3-q_1^0x_1^0+\mathbf{q}_1\mathbf{x}_1\right]}G\left(x_3, x_1\right). \tag{8.105}$$

Performing the first limit $x_1 \to -\infty$ we get

$$\sqrt{\frac{2q_3^0}{V}} \lim_{x_3^0\to\infty} \int d^3x_3 \;\; e^{iq_3x_3}e^{-iq_1x_3}\frac{1}{\sqrt{2q_1^0V}} = \lim_{x_3^0\to\infty} e^{i(q_3^0-q_1^0)x_3^0}\delta_{\mathbf{q}_3\mathbf{q}_1} = \delta_{\mathbf{q}_3\mathbf{q}_1} \tag{8.106}$$

which is just the scalar product

$$\langle\mathbf{q}_3|\mathbf{q}_1\rangle = \langle 0|a_{\mathbf{q}_3}a^\dagger_{\mathbf{q}_1}|0\rangle = \delta_{\mathbf{q}_3,\mathbf{q}_1} \tag{8.107}$$

of the particle 1 running from the initial to the final state 2 without interaction. The same factor appears for the lower line of the diagram

$$\langle\mathbf{q}_4|\mathbf{q}_2\rangle. \tag{8.108}$$

Thus the diagram turns into the S matrix element

$$\delta_{\mathbf{q}_3\mathbf{q}_1}\delta_{\mathbf{q}_2\mathbf{q}_4}. \tag{8.109}$$

The second diagram results in the same product of δ-functions except with $\mathbf{q}_3$ and $\mathbf{q}_4$ interchanged. The third diagram is different. Here the Fourier limit to be done is

$$\sqrt{\frac{2q_1^0}{V}}\sqrt{\frac{2q_2^0}{V}} \lim_{t_1<t_2\to-\infty} \int d^3x_1 d^4x_2^3 e^{-i\left[q_2^0x_2^0-\mathbf{q}_2\mathbf{x}_2-q_1^0x_1^0+\mathbf{q}_1\mathbf{x}_1\right]}G(x_2, x_1). \tag{8.110}$$

The first limit on x_1 leads to

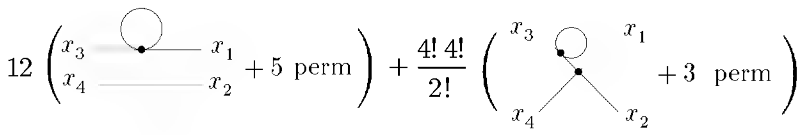
$$\sqrt{\frac{2q_2^0}{V}} \lim_{t_2 \to -\infty} \int d^3x_2 e^{-iq_2x_2 - iq_1x_2} \frac{1}{\sqrt{2q_1^0 V}} \tag{8.111}$$

and the integration gives

$$\lim_{x_2 \to -\infty} e^{-i(q_2^0+q_1^0)x_2^0} \delta_{\mathbf{q}_2,-\mathbf{q}_1}. \tag{8.112}$$

The limit $x_0 \to -\infty$ of the exponential oscillates infinitely rapid and the result vanishes for the same reasons as before.

Let us now look at the diagrams



in (8.63). The two rightmost contributions vanish since they pick up a factor (8.112). The other four are permutations of the left upper diagram From the lower line this obviously gives a factor

$$\langle \mathbf{q}_4 | \mathbf{q}_2 \rangle = \delta_{\mathbf{q}_4\mathbf{q}_2} \tag{8.113}$$

just as in (8.106). The upper line corresponds to the expression

$$12\left(-\frac{iq}{4!}\right) \int d^4z \;\; G(x_3, z)G(z, z)G(z_1, x_1) \tag{8.114}$$

and leads with the rules (8.101), (8.102) to

$$-i\frac{g}{2}\frac{1}{\sqrt{2Vq_2^0 2Vq_1^0}} \int d^4z \;\; e^{i(q_3-q_1)z} \int \frac{d^4q}{(2\pi)^4} \frac{i}{q^2-m^2} = -i\frac{g}{2}\delta_{\mathbf{q}_3\mathbf{q}_1}\frac{T}{2q_1^0} \int \frac{d^4q}{(2\pi)^4}\frac{i}{q^2-m^2}. \tag{8.115}$$

where T is the total time of the spacetime box in which the system is included. This diagram presents a modification of the expression (8.109) by a factor

$$1 - i\frac{g}{2}\frac{T}{2q_1^0} \int \frac{d^4q}{(2\pi)^4}\frac{i}{q^2-m^2} \tag{8.116}$$

where we have used the fact that the $2\pi\delta^{(1)}(q^0)$ function in energy equals T. The physical meaning of the factor (8.116) is a change of the mass of the particle in the presence of interactions. We shall see that it can be eliminated by taking the limits of infinite time not with the mass m appearing in the Lagrangian but rather with a renormalized mass value m_R.

To study such mass shifts in general we make use of the Gell-Mann Low formula for the energy shift. For the vacuum, the energy shifts by ΔE_0 can be taken from the matrix element

$$e^{-i\Delta E_0(t_2-t_1)} = \langle 0|U_I^\eta\left(t_2,t_1\right)|0\rangle \tag{8.117}$$

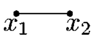
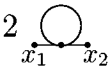
by going to the limit $t_2 \to \infty$, $t_1 \to -\infty$. Consider now the single-particle state $a_{\mathbf{q}}^\dagger|0\rangle$. If the interaction is applied, the state

$$U_I^\eta\left(t_2,t_1\right)a_{\mathbf{q}}^\dagger|0\rangle \tag{8.118}$$

will for $t_1 \to -\infty$ and $t_2 \to \infty$ again be a solution of the free Hamiltonian. Because of energy and momentum conservation, it must be equal to $a_{\mathbf{q}}^\dagger|0\rangle$ up to a phase which, due to (8.117), contains the information on the energy shift of this state. It consists of ΔE_0 for the vacuum plus $\Delta E_{\mathbf{q}}$ for the particle. Collecting both together in ΔE we may write

$$e^{-\Delta E(t_1-t_0)} \underset{\substack{t_1\to\infty\\ t_2\to-\infty}}{=} \langle 0|a_{\mathbf{q}}U_I^\eta\left(t_2t_1\right)a_{\mathbf{q}}^\dagger|0\rangle/\langle 0|U_I^\eta\left(t_2,t_1\right)|0\rangle. \tag{8.119}$$

Expanding U_I^η in powers of g, the lowest diagrams on the right-hand side are precisely the diagrams which appeared before:

$G^{(2)}(x_1,x_2) =$  $+\,12$  $+$

Indeed, we find with $t_1 - t_0 = T$

$$\begin{aligned}
1 - i\Delta E T &= 1 + 12\left(\frac{-ig}{4!}\right)\frac{1}{2q^0V}\int d^4z \;\; G(z_1,z)\\
&= 1 - \frac{i}{2}g\frac{T}{2q^0}\int\frac{d^4q}{(2\pi)^4}\frac{i}{q^2-m^2}
\end{aligned} \tag{8.120}$$

Thus, if we use in formula (8.95) the shifted energy $q^0 \to q^0 + \Delta E = q_R^0$ and write them as

$$\begin{aligned}
a_{\mathbf{q}}^\dagger &= \lim_{x^0\to-\infty}\sqrt{\frac{2q_R^0}{V}}\int d^3x e^{i(q_R^0x^0-\mathbf{qx})}\phi(x),\\
a_{\mathbf{q}} &= \lim_{x^0\to\infty}\sqrt{\frac{2q_R^0}{V}}\int d^3x e^{-i(q_R^0x^0-\mathbf{qx})}\phi(x),
\end{aligned} \tag{8.121}$$

then every particle line automatically receives a factor $e^{i\Delta E_qT}$ which precisely removes the phase factor (8.117).

If we want to go to higher orders in g, it is somewhat hard to proceed in this fashion The problem will be solved in the next section with more elegance.

Let us conclude by remarking that formula (8.119) allows to evaluate the shift in the particle mass. If $q^0=\sqrt{\mathbf{q}^2+m^2}$ is the energy before turning on the interaction and

$$q^0+\Delta E=\sqrt{\mathbf{q}^2+(m+\Delta m)^2}=q^0+\frac{m\Delta m}{q^0} \tag{8.122}$$

afterwards, we see by comparison with (8.120) that

$$\Delta m=\frac{g}{4}\int\frac{d^4q}{(2\pi)^4}\frac{i}{q^2-m^2} \tag{8.123}$$

8.8 Wick Rules for Scattering Amplitudes

The possibility of obtaining external particle states from fields by temporal limiting procedures of the type (8.95) allows us to incorporate the cration and annihilation ooperators of these particles into the general framework of Wick's contraction rules. Confronted with the numerator of the perturbative scattering amplitude in (8.91),

$$S_N\left(\mathbf{q}_4\mathbf{q}_3|\mathbf{q}_1\mathbf{q}_2\right)\;\equiv\;\langle 0|a_{\mathbf{q}_4}a_{\mathbf{q}_3}Te^{-i\int_{-\infty}^{\infty}dtV_I(t)}a^\dagger_{\mathbf{q}_2}a^\dagger_{\mathbf{q}_1}|0\rangle, \tag{8.124}$$

we may imagine the incoming particle operators to carry negative infinite time arguments, the outgoing ones positive infinite ones. Then they can be brought inside the parentheses of the time-ordering operator. This, in turn, can be evaluated as usual via Wick contractions.

The results of the last section show that the contractions leading to an external particles are

$$\begin{aligned}\dot\phi(x)\dot a^\dagger_{\mathbf{p}} &= [\dot\phi(x),\dot a^\dagger_{\mathbf{p}}]=\frac{1}{\sqrt{2V\omega_{\mathbf{p}}}}e^{-iqx},\\ \dot a_{\mathbf{p}}\dot\phi(x) &= [\dot a_{\mathbf{p}},\dot\phi(x)]=\frac{1}{\sqrt{2V\omega_{\mathbf{p}}}}e^{iqx},\end{aligned} \tag{8.125}$$

where $\omega_{\mathbf{p}}=\sqrt{\mathbf{p}+M^2}$.

For Dirac particles, there are corresponding rules

$$\begin{aligned}\dot\psi(x)\dot a^\dagger_{\mathbf{p},s_3} &= \{\dot\psi(x),\dot a^\dagger_{\mathbf{p},s_3}\}=\frac{1}{\sqrt{VE_{\mathbf{p}}}}u(\mathbf{p},\mathbf{s_3})e^{-ipx},\\ \dot a_{\mathbf{p},s_3}\dot{\bar\psi}(x) &= \{\dot a_{\mathbf{p},s_3},\dot{\bar\psi}(x)\}=\frac{1}{\sqrt{VE_{\mathbf{p}}}}e^{ipx}\bar u(\mathbf{p},\mathbf{s_3}),\end{aligned} \tag{8.126}$$

and for antiparticles:

$$\begin{aligned}\dot{\bar\psi}(x)\dot b^\dagger_{\mathbf{p},s_3} &= \{\dot{\bar\psi}(x),\dot b^\dagger_{\mathbf{p},s_3}\}=\frac{1}{\sqrt{VE_{\mathbf{p}}}}e^{-ipx}\bar v(\mathbf{p},\mathbf{s_3}),\\ \dot b_{\mathbf{p},s_3}\dot\psi(x) &= \{\dot b_{\mathbf{p},s_3},\dot\psi(x)\}=\frac{1}{\sqrt{VE_{\mathbf{p}}}}v(\mathbf{p},\mathbf{s_3})e^{ipx},\end{aligned} \tag{8.127}$$

where $E_{\mathbf{p}} \equiv \sqrt{\mathbf{p} + M^2}$.

8.9 Thermal Perturbation Theory

Since Wick's theorem was valid for thermal Green functions, we expect also the perturbation expansion to have a simple generalization to the thermal case. Let us define a thermal Heisenberg picture for operators by

$$O_H(\tau) = e^{H\tau/\hbar} O_S e^{-H\tau/\hbar} \tag{8.128}$$

and an interaction picture which moves according to the free equations of motion,

$$O_I(\tau) = e^{H_{0G}\tau/\hbar} O_S e^{-H_{0G}\tau/\hbar}. \tag{8.129}$$

Thus, a Heisenberg operator can be transformed to the free operator via

$$O_H(\tau) = U_I(0,\tau) O_I(\tau) U_I(\tau,0) \tag{8.130}$$

where

$$U_I(\tau_2,\tau_1) = e^{H_{0G}\tau_2/\hbar} e^{-H_G(\tau_2-\tau_1)} e^{-H_{0G}\tau_1/\hbar} \tag{8.131}$$

is the time displacement operator along the euclidean time axis τ. Therefore it has the same factorization property as the quantum mechanical operator $U_I(t_2,t_1)$,

$$U_I(\tau_3,\tau_2) U_I(\tau_2,\tau_1) = U(\tau_3,\tau_1). \tag{8.132}$$

Certainly

$$U_I(\tau_1,\tau_1) = 1. \tag{8.133}$$

The operator is not unitary but satisfies

$$U(\tau_2,\tau_1)^\dagger = U(-\tau_1,-\tau_2). \tag{8.134}$$

It obeys the following equation of motion

$$\begin{aligned} \hbar\partial_\tau U_I(\tau,\tau') &= e^{H_0\tau/\hbar}\left(H_{0G} - H_G\right) e^{-H_G(\tau-\tau)/\hbar} e^{-H_{0G}\tau/\hbar} \\ &= -V_I\, U(\tau,\tau') \end{aligned} \tag{8.135}$$

where V_I is now the thermal interaction picture of the time independent Schrödinger perturbation $V = V_S$

$$V_I(\tau) = e^{H_{0G}\tau/\hbar} V e^{-H_{0G}\tau/\hbar}. \tag{8.136}$$

Therefore we can solve for U via the standard exponential Neumann-Liouville expansion, now ordered with respect to the euclidean time τ:

$$\begin{aligned} U_I(\tau,\tau') &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2 \dots \int_{\tau'}^{\tau} d\tau_n T_T \left[V_I(\tau_1)\cdots V_I(\tau_n)\right] \\ &= T_\tau e^{-\frac{1}{\hbar}\int_{\tau'}^{\tau} d\tau'' V_I(\tau'')}. \end{aligned} \tag{8.137}$$

By construction, U_I satisfies the relation

$$e^{-H_G\tau/\hbar} = e^{-H_0\tau/\hbar}U(\tau,0). \tag{8.138}$$

Thus, using $\tau/\hbar = 1/k_BT$ we obtain directly a perturbation expansion of the partition function

$$\begin{aligned} Z &= \mathrm{Tr}\left(e^{-H_G/k_BT}\right) = \mathrm{Tr}\left(e^{-H_{0G}/k_BT}U\left(\frac{\hbar}{k_BT},0\right)\right) \qquad (8.139)\\ &= \sum_{n=0}^{\infty}\left(-\frac{1}{\hbar}\right)^n\frac{1}{n!}\int_0^{\frac{\hbar}{k_BT}}d\tau_1\cdots\int_0^{\frac{\hbar}{k_BT}}d\tau_n\mathrm{Tr}\Big(e^{-H_{0G}/k_BT}T_\tau\left(V_I(\tau_1)\cdots V_I(\tau_n)\right)\Big). \end{aligned}$$

Consider now a thermal two-body Green function in the presence of interaction which is defined for $\tau > \tau'$ as

$$\begin{aligned} G(\mathbf{x}\tau,\mathbf{x}'\tau') &\equiv \mathrm{Tr}\left[e^{-H_G/k_BT}\psi(\mathbf{x},\tau)\psi^\dagger(\mathbf{x}',\tau')\right]/\mathrm{Tr}\left[e^{-H_G/k_BT}\right]\\ &= \mathrm{Tr}\left[e^{-H_{0G}/k_BT}U_I\left(\frac{\hbar}{k_BT},0\right)U_I(0,\tau)\psi_I(\mathbf{x},\tau)U_I(\tau,0)\right. \qquad (8.140)\\ &\qquad\left.\times U(0,\tau')\psi_I^\dagger(\mathbf{x}',\tau')U(\tau',0)\right]/\mathrm{Tr}\left[e^{-H_{0G}/k_BT}U\left(\frac{\hbar}{k_BT},0\right)\right]. \end{aligned}$$

For $\tau < \tau'$, on the other hand, we have

$$\begin{aligned} G(\mathbf{x}\tau,\mathbf{x}'\tau') &\equiv \pm\mathrm{Tr}\left[e^{-H_G/k_BT}\psi^\dagger(\mathbf{x}',\tau')\psi(\mathbf{x},\tau)\right]/\mathrm{Tr}\left[e^{-H_G/k_BT}\right]\\ &= \mathrm{Tr}\left[e^{-H_{0G}/k_BT}U_I\left(0,\tau'\right)\psi_I^\dagger(\mathbf{x}',\tau')U_I(\tau',0)\right. \qquad (8.141)\\ &\qquad\left.\times U_I(0,\tau)\psi_I(\mathbf{x},\tau)U(\tau,0)\right]/\mathrm{Tr}\left[e^{-H_{0G}/k_BT}U\left(\frac{\hbar}{k_BT},0\right)\right]. \end{aligned}$$

Both equations may be combined in the single formula

$$\begin{aligned} G(\mathbf{x}\tau,\mathbf{x}'\tau') &= \mathrm{Tr}\left[e^{-H_{0G}/k_BT}T_\tau U\left(\frac{\hbar}{k_BT},0\right)\psi(x,\tau)\psi^\dagger\left(\mathbf{x}',\tau'\right)\right]\\ &\qquad /\mathrm{Tr}\left[e^{-H_{0G}/k_BT}U\left(\frac{\hbar}{k_BT},0\right)\right]. \qquad (8.142) \end{aligned}$$

As compared with the field theoretic case, the vacuum expectation is replaced by the weighted trace and the S matrix operator $U(\infty,-\infty)$ by the finite U_I operator $U_I(\hbar/k_BT,0)$ along the euclidean time axis τ. We can now expand U_I in powers of the interaction just as before and arrive at a thermally averaged product of many fields ψ_I which move according to the free field equations. Therefore Wick's theorem can be applied and we obtain an expansion of $G(\mathbf{x}\tau,\mathbf{x}'\tau')$ completely analogous to the field theoretic one. The only difference is the finite time interaction. When going to Fourier transformed space, the finite euclidean time interval corresponds to, and is fully taken into account by, the discrete set of imaginary Matsubara frequencies.

We have seen before that the evaluation fo field theoretic Green function proceeds best via a Wick rotation of the energy interactions to imaginary axis. This is precisely the axis along which the Matsubara frequencies lie. Thus as far as perturbation theory in Fourier transformed space is concerned, the diagrammatic rules are exactly the same except that the Wick rotated integrals over the imaginary energy are to be replaced by frequency sums

$$\int \frac{dp^0}{2\pi} \to i \int_{-\infty}^{\infty} \frac{dp_E}{2\pi} \to \frac{k_B T}{\hbar} \sum_{\omega_n}, \qquad \omega_n = 2\pi \begin{cases} n & \text{bosons} \\ n+\frac{1}{2} & \text{fermions.} \end{cases} \tag{8.143}$$

In the limit of small temperature, the Matsubara frequencies move closer and closer and the sum tends to the integral. The two descriptions coincide apart from the trivial presence of the chemical potential in the grand canonical energy. We conclude that the Wick rotated calculation of field theoretic Green function really amounts to thermal equilibrium physics in the limit of zero temperature. Note that the definition of a thermal average automatically contains, in the denominator, an expression analogous to the phase factor $\langle 0|U(\infty, -\infty)|0\rangle$ at the field theoretic formula. This division ensures the existence of the zero temperature limit in just the same way as the phase factor did in the switching on limit $\eta \to 0$. In fact, the grand canonical partition function in the denominator may be written as

$$Z_G = e^{\Omega/k_B T} = \sum_n e^{-(E_n - \mu N_n)/k_B T} \tag{8.144}$$

such that in the limit $T \to 0$ it becomes a pure exponential for the ground state energy

$$Z_G \underset{T\to 0}{\longrightarrow} e^{-(E_0 - \mu N_0)/k_B T} \to e^{\pm\infty}. \tag{8.145}$$

This is the analogue of the infinitive phase factor for the field theoretic denominator.

Let us point out that the result (8.142) implies the same periodicity in $\hbar/k_B T$ of the full Green function $G(\mathbf{x}\tau, \mathbf{x}'\tau')$ as in the free case. First, we observe that due to the time independence of the Hamiltonian, there is now translational invariance in euclidean time T such that $G(\mathbf{x}\tau, \mathbf{x}'\tau')$ depends only on the difference $\tau - \tau'$:

$$\begin{aligned} G\left(\mathbf{x}\tau, \mathbf{x}'\tau'\right) &= \mathrm{Tr}\left[e^{-H_G\left(\frac{1}{k_B T} - \frac{\tau}{\hbar}\right)} \psi(\mathbf{x}, 0) e^{-H_G \frac{\tau-\tau'}{\hbar}} \psi^\dagger(\mathbf{x}', 0) e^{-H_G \tau'/\hbar}\right] / .\mathrm{Tr}\left[e^{-H_G/k_B T}\right] \\ &= \mathrm{Tr}\left[e^{-H_G(1/k_B T - \tau - \tau'/\hbar)} \psi(\mathbf{x}, 0) e^{-H_G \tau - \tau'/\hbar} \psi^\dagger(\mathbf{x}', 0)\right] / \mathrm{Tr}\left[e^{-H_G/k_B T}\right] \end{aligned} \tag{8.146}$$

Similarly, we conclude the dependence only on $\mathbf{x} - \mathbf{x}'$ by translational invariance in space, using $\psi(\mathbf{x}, \tau) = e^{i\mathbf{P}\mathbf{x}/\hbar} \psi(\mathbf{0}, \tau) e^{-i\mathbf{P}\mathbf{x}/\hbar}$ with the momentum operator $\mathbf{P}$. Thus we may write

$$G\left(\mathbf{x}\tau, \mathbf{x}'\tau'\right) = G(\mathbf{x} - \mathbf{x}', \tau - \tau'), \tag{8.147}$$

just as for the field theoretic Green functions in the vacuum. Now it is easy to see the periodicity. Take $-\hbar/k_BT < \tau - \tau' < 0$ and calculate

$$\begin{aligned}
G\left(\mathbf{x}-\mathbf{x}',\tau-\tau'\right) &= \pm\mathrm{Tr}\left[e^{-H_G/k_BT}\psi^\dagger(x',\tau')\psi(x,\tau)\right]/\mathrm{Tr}\left[e^{-H_G/k_BT}\right]\\
&= \pm\mathrm{Tr}\left[\psi(\mathbf{x},\tau)e^{-H_G/k_BT}\psi^\dagger(\mathbf{x}',\tau')\right]/\mathrm{Tr}\left[e^{-H_G/k_BT}\right]\\
&= \pm\mathrm{Tr}\left[e^{-H_G/k_BT}\psi\left(\mathbf{x},\tau+\frac{\hbar}{k_BT}\right)\psi^\dagger(\mathbf{x}',\tau')\right]/\mathrm{Tr}\left[e^{-H_G/k_BT}\right]\\
&= \pm G\left(\mathbf{x}-\mathbf{x}',\tau-\tau'+\frac{\hbar}{k_BT}\right)
\end{aligned} \tag{8.148}$$

which proves that interacting Boson and Fermi thermal Green functions are periodic and antiperiodic in $\hbar/k_BT$ for $\tau-\tau' \in (0, 2\hbar/k_BT)$, just as in the free case.

9

Extracting Finite Results from Perturbation Series. Regularization and Renormalization

The Feynman integrals introduced in the last chapter suffer from a serious defect: They are almost always divergent. Fortunately, there exists a certain class of field theories, called *renormalizable field theories*, for which it is nevertheless possible to extract finite predictions for physically observable quantities. All infinities can be absorbed into a few divergent prefactors in relations between input parameters of the theory and their observed physical values. The price to pay is the impossibility of predicting these parameters, but all other observable properties of the theory can be expressed in terms of their physical values. Typically, these parameters are masses and coupling constants, and the normalization of field operators.

The action of a scalar field with a ϕ^4-interaction in four dimensions defines such a renormalizable field theory and presents a very good demonstration object for this procedure. It will now be discussed in detail.

9.1 Vacuum Diagrams

The Lagrangian of the theory is

$$\mathcal{L} = \frac{1}{2}\left(\partial\phi\right)^2 - \frac{m^2}{2}\phi^2 - \frac{g}{4!}\phi^4, \tag{9.1}$$

so that there are lines

$$\text{———} \quad = \quad \frac{i}{q^2 - m^2}, \tag{9.2}$$

and vertices

$$\times \quad = \quad -\frac{g}{4!}. \tag{9.3}$$

The perturbation series for the Green functions

$$\begin{aligned} G^{(n)}\left(x_1, \cdots, x_n\right) &= \langle 0|Te^{-i\frac{g}{4!}\int dx\phi^4(x)}\phi(x_1)\ldots\phi(x_n)|0\rangle/\langle 0|Te^{-i\frac{g}{4!}\int dx\phi^4(x)}|0\rangle \\ &\equiv G^{(n)}_N(x_1, \ldots, x_n)/Z[0] \end{aligned} \tag{9.4}$$

is obtained by expanding numerator and denominator on the right-hand side in powers of the coupling constant g and performing all Wick contractions in the resulting time-ordered products of free-field operators. The dominator is a pure phase factor $e^{2i\phi^{\eta}_{\pm}}$, as we know from the Gell-Mann-Low formula (??). Its diagrammatic expansion has been given in Section 8.3.1, where it was shown to consist of a sum of all vacuum graphs. Here we are interested in the size of the individual terms. Using translational invariance in space and time, we may rewrite (8.34) as

$$\begin{aligned} Z[0] &= \langle 0|Te^{-i\frac{g}{4!}\int dx\phi^4(x)}|0\rangle \\ &= 1-iVT\left\{\frac{g}{4!}\langle 0|\phi^4(0)|0\rangle-\frac{1}{2!}\left(\frac{g}{4!}\right)^2\int dx\langle 0|\phi^4(x)\phi^4(0)|0\rangle+\dots\right\}. \end{aligned} \tag{9.5}$$

This expansion runs into an immediate difficulty: the first-order term does not exist in an infinite spacetime volume.[1] This difficulty can be avoided by continuing the discussion for a finite system in a finite time interval.

This, however, is not yet enough to produce finite results on the right-hand side of (9.5). Consider the first-order Feynman integral (8.36) in more detail. In momentum space it reads

$$-3i\frac{g}{4!}VT\left(\int\frac{d^4g}{(2\pi)^4}\frac{i}{q^2-m^2+i\eta}\right)^2 \tag{9.6}$$

where 3 is the multiplicity factor of the diagram. Performing the Wick rotation of Fig. 5.2, the mass shell singularity in the energy integral lies no longer on th eintegration contour, so that the $i\eta$-term may be omitted, and (9.6) is expressed in terms of a euclidean integral:

$$-i\frac{g}{4!}VT\left(\int\frac{d^4q_E}{(2\pi)^4}\frac{1}{q_E^2+m^2}\right)^2. \tag{9.7}$$

The integral has a quadratic divergence at large momenta. In order to obtain a finite result we have to modify the system in such a way that in addition to the finite spacetime volume VT, its Wick rotated energy-momentum space is finite as well. Thus we restrict all euclidean momenta q_E to lie within a sphere of rasius Λ:

$$q_E^2\leq\Lambda^2. \tag{9.8}$$

The integration radius Λ is called an *ultraviolet cutoff*, or shorter *UV cutoff*, since it eliminates the very short wavelengths of the field. Such an UV-cutoff would have arisen naturally if the physical phenomena would take place on a 4-dimensional lattice with spacing of the order $l=\pi/\Lambda$ between the lattice points rather than a continuous spacetime. On such a lattice, each term in the perturbation expansion would have a finite value. If the lattice spacing can be chosen much finer than the regions explored by presently available experiments, this would not present any practical handicap. Any perturbation expansion containing an UV-cutoff is of course unable to describe the physics going on between the lattice points.

---

[1] Recall that a similar overall time factor T was found before in the general discussion in Chapter 7. There it appeared in the limit that the switching-on parameter η tended to zero [see (7.95)]. In that general derivation we did not find a spatial volume factor, since in that chapter dealt with quantum mechanics, and not with a local quantum field theory.

Hopefully, this is a purely technical problem. If we could resum infinitely many diagrams, the series might define a function which can be used also beyond the cutoff (9.8). The simplest model function to illustrates such a hope is given by, say,

$$\left(\frac{q^2}{\mu^2}\right)^g. \tag{9.9}$$

where μ is some characteristic mass parameter of the problem. In a perturbation expansion, this function would appear as a series

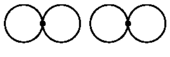
$$\sum_{n=1}^{\infty} g^n \left[\log(q^2/\mu^2)\right]^n. \tag{9.10}$$

This expansion makes sense only if the momenta of the system are contained within a sphere (9.8) whose size is smaller than

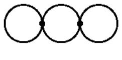
$$\Lambda^2 = \mu^2 e^{1/g}. \tag{9.11}$$

The unexpanded expression (9.9), on the other hand, is defined in the entire complex q^2-plane, except for a cut from $q^2 = 0$ to $-\infty$. This characteristic behaviour will indeed emerge in some partial resummation procedures of many perturbation series. In general, however, the divergences may be of a much more violent nature. The coefficients of the higher-order terms grow in general with $n!$, and the series have a zero radius of convergence. The physical significance of this violent divergence will be discussed later.

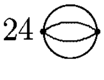
To second order in g, the Wick expansion of the second expectation value on the right-hand side of (9.5) yields the Feynman integrals (8.42). In momentum space they read



$$\frac{1}{2!}9 \qquad = \frac{1}{2!}9\left(\frac{g}{4!}\right)^2\left[\int đ^4q\frac{1}{q^2-m^2+i\eta}\right]^4,$$



$$\frac{1}{2!}72 \qquad = \frac{1}{2!}72\left(\frac{g}{4!}\right)^2\left[\int đ^4q_1\frac{i}{q_1^2-m^2+i\eta}\right]^2\int đ^4q_2\left(\frac{i}{q_2^2-m^2+i\eta}\right)^2, \tag{9.12}$$



$$\frac{1}{2!}24 \qquad = \frac{1}{2!}24\left(\frac{g}{4!}\right)^2\int đ^4q_1 đ^4q_2 đ^4q_3\frac{i}{q_1^2-m^2+i\eta}\frac{i}{q_2^2-m^2+i\eta}\frac{i}{q_3^2-m^2+i\eta}.$$

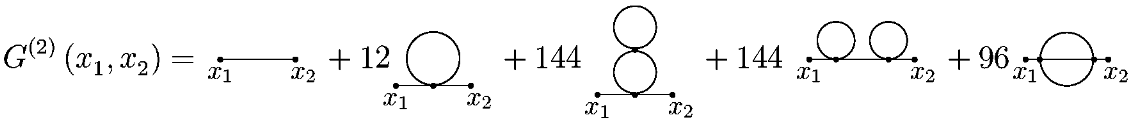
After performing again Wick rotations and introducing the euclidean momentum cutoff (9.8), we see that these expressions diverge as $\Lambda^8, \Lambda^4\log\Lambda, \Lambda^4$ respectively. Analogous statements hold for higher orders.

Thus the infinite phase caused by the vacuum diagrams diverges quite catastrophically for two reasons, both deriving from fundamental properties of spacetime: one is homogeneity (i. e., translational invariance) which causes the overall factors VT. The other is continuity of spacetime, which causes the Fourier representations fields to contain euclidean momentum integrals over an infinite momentum volume. It is a pleasant feature of the Gell-Mann-Low formula, that the divergence of the phase due to the vacuum diagrams is irrelevant. In Section 7.1 it was demonstrated that the phase in the denominator cancels against an identical phase arising in the numerator when expanding (9.4) in powers of g [recall (8.12)]. In terms of graphs this amounts to a cancellation of all Feynman diagrams in the numerator which contain a disconnected part occuring in the vacuum diagrams of the denominator. This cancelation removes all vacuum diagrams from the numerator, together with their unpleasant VT- and Λ-divergences. In quantum mechanics, this was sufficient to obtain finite results in the limit of a vanishing switching-on parameter μ.

We are thus confronted with only those Feynman graphs which are free of vacuum contributions. Consider the corresponding two- and four-point functions.

9.2 The Two- and Four-Point Functions

In Eq. (8.62) we have derived the first terms of the perturbation series for the two-point function:

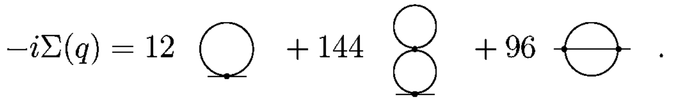


(9.13)

which amounts to the geometric series (8.73) in momentum space:

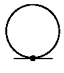
$$
\begin{aligned}
G^{(2)}(q) &= \frac{i}{q^2-m^2-\Sigma(q)} \qquad (9.14)\\
&= G_0(q)+G_0(q)\,[-i\Sigma(q)]\,G_0(q)+G_0(q)\,[-i\Sigma(q)]\,G_0(q)\,[-i\Sigma(q)]\,G_0(q)+\dots\,,
\end{aligned}
$$

with $\Sigma(q)$ being the sum of proper self-energy diagrams (= one-particle irreducible diagrams with two amputated legs)

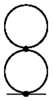


(9.15)

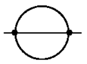
The Feynman integrals associated with these diagrams can be written in momentum space as follows:



$$
= -\frac{ig}{4!}\int \bar{d}^4k\,\frac{i}{k^2-m^2+i\eta},
$$



$$= \left(-\frac{ig}{4!}\right)^2 \int \bar{d}^4k_1 \left(\frac{i}{k_1^2-m^2+i\eta}\right)^2 \int \bar{d}^4k_2 \,\frac{i}{k_2^2-m^2+i\eta}, \tag{9.16}$$

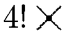
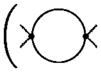


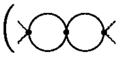
$$= \left(-\frac{ig}{4!}\right)^2 \int \bar{d}^4k_2\, \bar{d}^4k_1 \,\frac{i}{k_1^2-m^2+i\eta}\,\frac{i}{k_2^2-m^2+i\eta}\,\frac{i}{(q-k_1-k_2)^2-m^2+i\eta}. \tag{9.17}$$

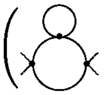
The four-point Green function is reduced to the vertex function $\Gamma^{(4)}$ by factorizing out the four Green functions:

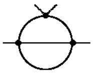
$$G^{(4)}(p_1,\dots,p_4) = G^{(2)}(p_1)G^{(2)}(p_2)G^{(2)}(p_3)G^{(2)}(p_4)i\Gamma^{(4)}(p_1,\dots,p_4). \tag{9.18}$$

The vertex function $i\Gamma^{(4)}$ collects all one-particle irreducible graphs with four amputated legs. [see (8.6.1) and (8.77)]. Up to third order:

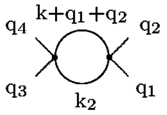
$i\Gamma^{(4)} = 4!$  $+ (4!)^2 \Big\{\frac{1}{2}\Big($  $+ 2\text{perm}\Big)\Big\}$

$+ (4!)^3 \Big\{\frac{1}{4}\Big($  $+ 2\text{perm}\Big)$

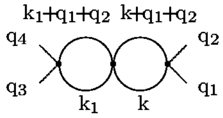
$+\frac{1}{2}\Big($  $+ 2\text{perm}\Big)$

$+\frac{1}{2}\Big($  $+ 5\text{perm}\Big)\Big\}.$ (9.19)

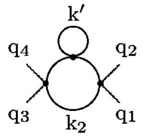
In momentum space, these graphs correspond to the Feynman integrals:



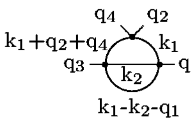
$$= \left(-\frac{ig}{4!}\right)^2 \int \bar{d}^4k \,\frac{i}{k^2-m^2+i\eta}\,\frac{i}{(k+q_1+q_2)^2-m^2+i\eta}, \tag{9.20}$$



$$= \left(-\frac{ig}{4!}\right)^3 \left[\int \bar{d}^4k \,\frac{i}{k^2-m^2+i\eta}\,\frac{i}{(k+q_1+q_2)^2-m^2+i\eta}\right]^2, \tag{9.21}$$



$$= \left(-\frac{ig}{4!}\right)^3 \int \bar{d}^4k \,\frac{i}{k^2-m^2+i\eta}\left[\frac{i}{(k+q_1+q_2)^2-m^2+i\eta}\right]^2 \times \int \bar{d}^4k \,\frac{i}{k'^2-m^2+i\eta}, \tag{9.22}$$



$$= \left(-\frac{ig}{4!}\right)^3 \int \bar{d}^4k_1\bar{d}^4k_2 \,\frac{i}{k_1^2-m^2+i\eta} \times \frac{i}{(k_1+q_2+q_4)^2-m^2+i\eta}\,\frac{i}{k_2^2-m^2+i\eta}\,\frac{i}{(k_1-k_2-q_1)^2-m^2+i\eta}. \tag{9.23}$$

We may perform the Wick rotation in the loop integrals so that now $\bar{d}^4q$ goes over into i times the euclidean volume elements $d^4q_E/(2\pi)^4$, and q^2 becomes $-q_E^2 = -(\mathbf{q}^2 + q_4^2)$. Then we find the following analytic expressions for self-energy and four-point vertex function:

$$\Sigma(q) = \frac{g}{2}D_1 - \frac{g^2}{4}D_2D_1 - \frac{g^2}{6}D_3(q), \tag{9.24}$$

$$\begin{aligned}\Gamma^{(4)}(q_i) \;=\; & g - \frac{g^2}{2}\left[I\left(q_1+q_2\right) + 2\text{ perm}\right] + \frac{g^3}{4}\left[I^2\left(q_1+q_2\right) + 2\text{ perm}\right] \\ & + \frac{g^3}{2}\left[I_3\left(q_1+q_2\right)D_1 + 2\text{ perm}\right] + \frac{g^3}{2}\left[I_4\left(q_i\right) + 5\text{ perm}\right].\end{aligned} \tag{9.25}$$

Here, $D_{1,2,3}$ and I are the following Feynman integrals

$$D_1 = \int \bar{d}^4k \frac{1}{k^2+m^2}, \tag{9.26}$$

$$D_2 = \int \bar{d}^4k \frac{1}{\left(k^2+m^2\right)^2}, \tag{9.27}$$

$$D_3(q) = \int \bar{d}^4k_1 \bar{d}^4k_2 \frac{1}{\left(k_1^2+m^2\right)\left(k_2^2+m^2\right)\left[(q-k_1-k_2)^2+m^2\right]}, \tag{9.28}$$

$$I(q) = \int \bar{d}^4k \frac{1}{\left(k^2+m^2\right)} \frac{1}{\left[(k+q)^2+m^2\right]}, \tag{9.29}$$

$$I_3(q) = \int \bar{d}^4k \frac{1}{\left(k^2+m^2\right)^2} \frac{1}{\left[(k+q)^2+m^2\right]}, \tag{9.30}$$

$$\begin{aligned}I_4(q_i) = & \int \bar{d}^4k_1 \bar{d}^4k_2 \frac{1}{\left(k_1^2+m^2\right)\left[(k_1+q_2+q_4)^2+m^2\right]} \\ & \times \frac{1}{\left(k_2^2+m^2\right)\left[(+k_1-k_2-q_1)^2+m^2\right]}.\end{aligned} \tag{9.31}$$

9.3 Divergences, Cutoff, and Counterterms

The trouble with these expressions is that, except for I_3, all integrals diverge. In order to extract physical information from them, we introduce an ultraviolet cutoff (9.8) and integrate all momenta only over a spherical range $q^2 \leq \Lambda^2$. Then for large Λ, the different expressions diverge like $D_{1,3} \sim \Lambda^2, D_2, I \sim \log\Lambda^2/m^2, I_4 \sim \log^2\Lambda^2/m^2$.

In the presence of such a cutoff we must watch out that the size of the coupling constant remains small enough to justify an expansions in powers of g. In the present case we have to require at first that the quantities

$$g\,\Lambda^2/m^2, \qquad g\,\log\Lambda^2/m^2, \qquad g^2\,\log^2\Lambda^2/m^2 \tag{9.32}$$

are all very much smaller than unity. As far as the first term is concerned, this severely restricts the size of g for narrow lattices with $\Lambda^2 \gg m^2$. The other contributions involving logarithms are not so restrictive and permit somewhat more sizable couplings, since the logarithm grows very slowly with Λ/m.

Before proceeding it is useful to separate each momentum integral into a term which diverges for $\Lambda \to \infty$, and a remainder which remains finite in this limit, and thus independent of Λ. A standard procedure do this consists in expanding the diverging integrals in a power series of the external momenta. Then we see that after a few diverging expansion terms all coefficients are finite. We collect the remaining finite powers and call this part the *regular part* of the diagram. For the diagrams under consideration the expansions read

$$D_3(q) = D_3(0) + D_3'(0)q^2 + D_3^R(q), \tag{9.33}$$

$$I(q) = I(0) + I^R(q), \tag{9.34}$$

where a prime denotes the derivative with respect to q^2. Only the initial expansion terms $D_3(0), D_3'(0), I(0)$ are divergent for $\Lambda \to \infty$. The remainders $D^R(q)$, $I^R(q)$ are cutoff-independent functions of the momenta.

The Feynman amplitude $I_4(q_i)$ involves two integrations. Since the expansion (9.25) contains all 6 permutations of the momenta q_1, q_2, q_3 (the fourth being fixed by energy-momentum conservation, $q^4 = -q_1 - q_2 - q_3$), we may freely permute the momenta in the integral (9.23) and calculate

$$I_4(q_i) = \int d^4k \frac{1}{(k^2+m^2)\left[(q_1+q_2-k)^2+m^2\right]} I\left(q_3+k\right) \tag{9.35}$$

where $I(q)$ is the integral (9.29), which is expanded as in (9.34). Thus we can write

$$I_4(q_i) = I(q_1+q_2)I(0) + \int d^4k \frac{1}{(k^2+m^2)\left[(q_1+q_2-k)^2+m^2\right]} I^R\left(q_3+k\right). \tag{9.36}$$

Performing the subtraction in $I\left(q_1+q_2\right)$ we have

$$\begin{aligned} I_4(q_i) &= I^2(0) + I^R(q_1+q_2)I(0) \\ &\quad + \int d^4k \frac{1}{(k^2+m^2)\left[(q_1+q_2-k)^2+m^2\right]} I^R\left(q_3+k\right). \end{aligned} \tag{9.37}$$

The last term can now be subtracted at $q_i = 0$, leaving a finite remainder. Since $I^R(0) = 0$, we may also write

$$I_4(q_i) = I_4(0) + I^R\left(q_1+q_2\right)I(0) + I_4^R(q_i). \tag{9.38}$$

There are two types of cutoff dependences: One which is momentum-independent and one which is accompanied by the regularized amplitude $I^R\left(q_1+q_2\right)$. This structure will be important in achieving a finite vertex function. With this separation we can rewrite Σ and $\Gamma^{(4)}$

$$\begin{aligned}
\Sigma(q) &= \Sigma(0)+\Sigma'(0)q^2+\Sigma^R(q), && (9.39)\\
\Gamma^{(4)}(q_i) &= g-\frac{g^2}{2}\left\{3I(0)+\left[I^R(q_1+q_2)+2\text{ perm}\right]\right\}\\
&+\frac{g^3}{4}\left\{3I^2(0)+2\left[I^R(q_1+q_2)+2\text{ perm}\right]I(0)+\left[(I^R(q_1+q_2))^2+2\text{ perm}\right]\right\}\\
&+\frac{g^3}{2}\left[I_3(q_1+q_2)+2\text{ perm}\right]D_1\\
&+\frac{g^3}{2}\left\{6I_4(0)+\left[I_4^R(q_i)+5\text{ perm}\right]\right\}, && (9.40)
\end{aligned}$$

with the Λ-dependent quantities

$$\begin{aligned}
\Sigma(0) &= \frac{g}{2}D_1-\frac{g^2}{4}D_2D_1-\frac{g^2}{6}D_3(0), && (9.41)\\
\Sigma'(0) &= -\frac{g^2}{6}D_3'(0). && (9.42)
\end{aligned}$$

Let us interprete this separation physically. For this we consider the full single-particle propagator (9.14). It has the form

$$G^{(2)}(q)=\frac{1}{q^2+m^2+\Sigma(0)+\Sigma'(0)q^2+\Sigma^R(q)}. \tag{9.43}$$

The pole of this propagator corresponds to the mass of the particle after the perturbative corrections. If the cutoff is sufficiently large we may, for a moment, neglect $\Sigma^R(q)$. Then $G^{(2)}$ can be rewritten as

$$\begin{aligned}
G^{(2)}(q) &= \frac{1}{q^2\left[1+\Sigma'(0)\right]+\left[m^2+\Sigma(0)\right]}\\
&= \frac{\left[1+\Sigma'(0)\right]^{-1}}{q^2+m^2\left[1+\Sigma(0)/m^2\right]/[1+\Sigma'(0)]}. && (9.44)
\end{aligned}$$

This looks like the propagator of a free field $\langle 0|T\phi_R(x)\phi_R(y)|0\rangle$, with

$$\phi_R\equiv\sqrt{1+\Sigma'(0)}\,\phi, \tag{9.45}$$

and a mass

$$m_R^2=m^2\frac{1+\Sigma(0)/m^2}{1+\Sigma'(0)}. \tag{9.46}$$

Experimentally, only the renormalized mass m_R is observable; there is no way of detecting the original mass parameter m in the Lagrangian.

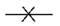
Thus, in all amplitudes calculated from the Lagrangian, the mass m_R has to be used in the final expression rather than m. Technically, this turns out to be slightly inconvenient. There is a more economic method due to Bogoljubov which is based on adding to the Lagrangian a set of counterterms which have the same form as the terms of the original Lagrangian. First the free parts:

$$\mathcal{L}_c = c^{\phi}\frac{1}{2}(\partial\phi)^2 - c^{m^2}\frac{m^2}{2}\phi^2. \tag{9.47}$$

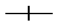
The coefficient functions are expanded in a power series in g starting with g:

$$c^{\phi} = \sum_{n=1}^{\infty} c_n^{\phi} g^n, \qquad c^{m^2} = \sum_{n=1}^{\infty} c_n^{m^2} g^n. \tag{9.48}$$

They are supposed to be small enough to be treated as a perturbation. If we now calculate the self-energy $\Sigma(q)$ up to order g^2 we find the additional OPI Feynman graphs

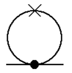


$$= \left(c_1^{m^2} g + c_2^{m^2} g^2 \right) m^2,$$

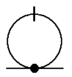


$$= \left(c_1^{\phi} g + c_2^{\phi} g^2 \right) p^2, \tag{9.49}$$

and loops of the form



$$= \tfrac{1}{2}\, c_1^{m^2} g^2 m^2 D_2,$$



$$= \tfrac{1}{2}\, c_1^{\phi} g^2 \int d^4k \frac{k^2}{\left(k^2+m^2\right)^2} = \frac{1}{2}\, c_1^{\phi} g^2 \left(D_1 - m^2 D_2\right). \tag{9.50}$$

The crosses and little circles are called *mass-* and *wave function insertions*, respectively. When adding these terms to the cutoff-dependent parts of the self-energy, they become

$$\begin{aligned} \Sigma^{\text{sg}}(q) \;=\; & \frac{g}{2}D_1 - \frac{g^2}{4}D_2 D_1 - \frac{g^2}{6}D_3(0) - \frac{g^2}{6}D_3'(0)\,q^2 \\ & + \left(c_1^{m^2} g + c_2^{m^2} g^2 \right) m^2 + \left(c_1^{\phi} g + c_2^{\phi} g^2 \right) q^2 \\ & + \frac{1}{2}\, c_1^{m^2} g^2 m^2 D_2 + \frac{1}{2}\, c_1^{\phi} g^2 \left(D_1 - m^2 D_2\right). \end{aligned} \tag{9.51}$$

The point is now that we can always choose the counterterms in such a way that the physical mass arrives at the value m we started out with. This can be done order by order in perturbation theory:

To order g we determine

$$c_1^{m^2} m^2 = -\frac{1}{2} D_1, \qquad c_1^\phi = 0. \tag{9.52}$$

Inserting this into (9.51), we see that the second and 9th term cancel each other. To second order we determine

$$\begin{aligned} c_2^{m^2} m^2 &= \frac{1}{6} D_3(0), \qquad (9.53)\\ c_2^\phi &= \frac{1}{6} D_3'(0). \qquad (9.54) \end{aligned}$$

With these choices, no cutoff-dependent parts are left in $\Sigma(q)$ and

$$\Sigma(q) \equiv \Sigma_R(q) = -\frac{g^2}{6} \left[D_3(q) - D_3(0) - D_3'(0) q^2 \right]. \tag{9.55}$$

As far as the physical results are concerned, this procedure is completely equivalent to the first. The only difference is that with the counterterms the original mass parameter in the Lagrangian winds up directly in the final expressions whereas in the first method all expressions must be brought to the renormalized form at the end of all calculations.

The counterterm method really means that instead of the original Lagrangian we have worked with the modified Lagrangian

$$\mathcal{L} + \mathcal{L}_c = \frac{1 + \ c^\phi}{2} (\partial \phi)^2 - \frac{1 + \ c^{m^2}}{2} m^2 \phi^2 \tag{9.56}$$

where ϕ and m are the renormalized field and masses, respectively. This is equivalent to starting out with

$$\mathcal{L}_0 \equiv \mathcal{L} + \mathcal{L}_c = \frac{1}{2} (\partial \phi_0)^2 - \frac{m_0^2}{2} \phi_0^2 \tag{9.57}$$

where

$$\phi_0 \equiv \sqrt{1 + \ c^\phi} \phi, \qquad m_0^2 \equiv m^2 (1 + \ c^{m^2})(1 + \ c^\phi)^{-1}. \tag{9.58}$$

Identifying this ϕ_0 with the previous ϕ and the new ϕ with the previous ϕ_R we see that to lowest order in $g c^\phi = -\Sigma'(0), \ \ c^{m^2} = -\Sigma(0)$. To higher orders, an additional change from m to m_R is necessary in the normalization factors (9.45), (9.46) for a comparison with the result (9.58) [the integrals $\Sigma(0), \Sigma'(0)$ in (9.41), (9.42) are expressed in terms of the unrenormalized mass, while c^ϕ, c^{m^2} in (9.54),(9.53) contain the renormalized mass].

The counterterm method has the obvious advantage that at every stage only cutoff-independent quantities appear in the calculated amplitudes.

Note that the physical mass is not quite equal to the Lagrangian parameter m^2. The propagator is

$$G^{(2)}(q) = \frac{1}{q^2 + m^2 + \Sigma_R(q)}, \tag{9.59}$$

and the renormalized quantity $\Sigma_R(q)$ will cause a shift of the pole position to order g in the coupling constant. This finite shift may, however, be easily calculated.

At this point we realize that the finite shift can also be avoided by expanding the loop integrals not around zero but around $q^2 = m^2$. Then

$$D_3(q) = D_3(q)|_{q^2=m^2} + (q^2 + m^2)D_3'(m^2) + \tilde{D}_3^R(q). \tag{9.60}$$

Now the counterterms would be (9.52), together with

$$c_2^{m^2} m^2 = -\frac{1}{6}\left[D_3(m^2) - m^2 D_3'(m^2)\right], \tag{9.61}$$

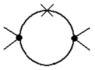
$$c_2^{\phi} = -\frac{1}{6} D_3'|_{q^2=-m^2}, \tag{9.62}$$

leading to a propagator

$$G^{(2)}(q) = \frac{1}{q^2 + m^2 + \tilde{\Sigma}_R(q)}, \tag{9.63}$$

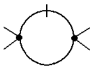
where the regular part starts out with the second power in $q^2 + m^2$ and therefore leaves the pole at its initial place $q^2 = -m^2$.

Consider now the four-point vertex $\Gamma^{(4)}$. To make it finite we have to include the additional graphs caused by the counterterms (9.47). The lowest contribution enters to order g^3:



$$= g^3 \;\; c_1^{m^2} m^2 \left[I_3\left(q_1 + q_2\right) + 2 \text{ perm}\right],$$

(9.64)



$$= g^3 \;\; c_1^{\phi} \left\{\left[I\left(q_1 + q_2\right) - m^2 I_3\left(q_1 + q_2\right)\right] + 2 \text{ perm}\right\}.$$

Using (9.52), this gives

$$-\frac{g^3}{2} D_1 \left[I_3\left(q_1 + q_2\right) + 2 \text{ perm}\right], \tag{9.65}$$

thus canceling the second-last line in (9.40).

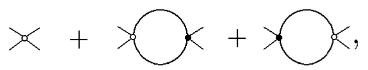
To regularize the remaining Λ-dependent quantities, we introduce a counterterm of the interaction type

$$\mathcal{L}_c = -\frac{g}{4!} c^g \, \phi^4 \tag{9.66}$$

where c^g has an expansion:

$$c^g = \sum_{n=1}^{\infty} c^g_n g^n. \tag{9.67}$$

This adds to the four-point vertex $\Gamma^{(4)}$ the diagrams



(9.68)

where the small circles denote the coupling constant counterterms. These insertions amount to replacing $g \to g\left(1 + c^g_1 g + c^g_2 g^2\right)$ in the first and second term of the expansion (9.40) (the others receive corrections $\mathcal{O}(g^4)$.

It remains to combine mass and coupling constant insertions. To order g^3, there are none. The corrected expression for $\Gamma^{(4)}$ is therefore

$$\begin{aligned}
\Gamma^{(4)} &= g\left(1 + c^g_1 g + c^g_2 g^2\right) \\
&- \frac{1}{2}\left(g^2 + 2\, c^g_1 g^3\right)\left\{3I(0) + \left[I^R(q_1+q_2) + 2\text{ perm}\right]\right\} \\
&+ \frac{g^3}{4}\left\{3I^2(0) + 2\left[I^R(q_1+q_2) + 2\text{ perm}\right]I(0) + \left[(I^R(q_1+q_2))^2 + 2\text{ perm}\right]\right\} \\
&+ \frac{g^3}{2}\left\{6I_4(0) + \left[I^R_4(q_i) + 5\text{ perm}\right]\right\}.
\end{aligned} \tag{9.69}$$

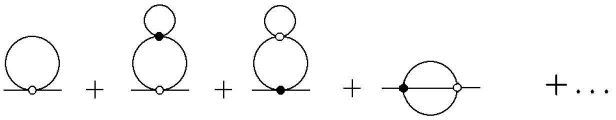
We now determine c^g order by order to cancel the remaining infinities:

$$\begin{aligned}
c^g_1 &= \frac{3}{2}I(0), \\
c^g_2 &= \frac{15}{4}I^2(0) - 3I_4(0).
\end{aligned} \tag{9.70}$$

The result is the renormalized $\Gamma^{(4)}$:

$$\begin{aligned}
\Gamma^{(4)}_R(q_i) = g &- \frac{g^2}{2}\left[I^R(q_1+q_2) + 2\text{ perm}\right] \\
&+ \frac{g^3}{4}\left[I^{R^2}(q_1+q_2) + 2\text{ perm}\right] + \frac{g^3}{2}\left[I^R_4(q_i) + 5\text{ perm}\right].
\end{aligned} \tag{9.71}$$

Finally, we have to consider the effects of the coupling constant counterterms upon the self energy. There are the additional graphs



(9.72)

of which only the first contributes to the second-order expression (9.51), with an amplitude

$$\frac{g^2}{2}\,c_1^g D_1 = \frac{3}{4}g^2 I(0) D_1.$$

Adding this to (9.51), the quadratic mass counterterm is modified to

$$c_2^{m^2} = \frac{1}{6}D_3(0) - \frac{3}{4}I(0)D_1. \tag{9.73}$$

In this way we have arrived at cutoff-independent expressions for Σ and $\Gamma^{(4)}$. Note, in particular, that the unpleasant terms in the vertex function (9.69) which depend on both, cutoff and momenta, have dropped out.

The total counterterms to second order in g are

$$\begin{aligned} c^{m^2} m^2 &= -\frac{1}{2}gD_1 + \frac{g^2}{6}D_3(0) - \frac{3}{4}g^2 I(0) D_1, &(9.74)\\ c^{\phi} &= \frac{1}{6}D_3'(0)g^2, &(9.75)\\ c^{g} &= g\frac{3}{2}I(0) + g^2\left[\frac{15}{4}I^2(0) - 3I_4(0)\right] - \frac{g^2}{3}. &(9.76)\end{aligned}$$

This procedure can be extended to any order in perturbation theory. Moreover, if more general vertex functions are calculated with an arbitrary number of legs the counterterms regularizing the two and four point vertices are sufficient to guarantee also their cutoff independence. The general argument will be formulated in the next chapter.

9.4 Bare Theory and Multiplicative Renormalization

There is one important aspect of the counterterms which has to be stressed: All counterterms have the same form as the terms in the original Lagrangian. Thus one may rewrite $\mathcal{L} + \mathcal{L}_c$ as

$$\mathcal{L} + \mathcal{L}_c = \frac{1+c^{\phi}}{2}\left(\partial\phi\right)^2 - \frac{1+c^{m^2}}{2}m^2\left(\partial\phi\right)^2 - \frac{g}{4!}\left(1+c^g\right)\phi^4. \tag{9.77}$$

Therefore we can return to the original form by a multiplicative renormalization. We define the so-called bare fields, mass, and coupling constant

$$\begin{aligned} \phi_B &\equiv \phi Z_{\phi}^{1/2} = \phi(1+c^{\phi})^{1/2}, &(9.78)\\ m_B^2 &= m^2 Z_m Z_{\phi}^{-1} = m^2(1+c^{m^2})/(1+c^{\phi}), &(9.79)\\ g_B &= gZ_g Z_{\phi}^{-2} = g_B(1+c^g)/(1+c^{\phi})^2. &(9.80)\end{aligned}$$

and the total Lagrangian becomes

$$\mathcal{L} + \mathcal{L}_c \equiv \mathcal{L}_B = \frac{1}{2}\left(\partial\phi_B\right)^2 - \frac{m_B^2}{2}\phi_B^2 - \frac{g_B}{4!}\phi_B^4. \tag{9.81}$$

In this bare Lagrangian, all quantities depend on the physical parameters m, g and the cutoff Λ. However, due to the renormalizability of the theory, all Λ-dependence drops out and only functions of m and g remain.

It is instructive to see the renormalization work if one uses the bare Lagrangian (9.81) as a basis for a perturbation expansion wihtout constructing counterterms order by order in g. Thus we calculate from the original graphs (9.15) and (9.19) the self-energy (9.24), (9.25), now expressed in terms of the bare parameters g_B and m_B instead of g, m. We find renormalized Green functions by multiplying the bare Green functions with a factor $Z_\phi^{-1/2}$ for each field,i.e.,

$$
\begin{aligned}
G_R^{(2)} &= Z_\phi^{-1} G_B, && (9.82)\\
G_R^{(4)} &= Z_\phi^{-2} G_B^{(4)}. && (9.83)
\end{aligned}
$$

The bare vertex functions

$$\Gamma_B^{(4)} \equiv G_B^{-1} G_B^{-1} G_B^{-1} G_B^{-1} G_B^{(4)}$$

become finite via the inverse factors

$$
\begin{aligned}
\Gamma_R^{(2)} &= \Gamma_B^{(2)} Z_\phi, && (9.84)\\
\Gamma_R^{(4)} &= \Gamma_B^{(4)} Z_\phi^2. && (9.85)
\end{aligned}
$$

In the previous scheme, the renormalized two-point vertex took the form

$$\Gamma_R^{(2)}(q) = q^2 + m^2 + \Sigma^R(q) \tag{9.86}$$

where m is the renormalized mass defined before. Thus we may identify m from

$$\Gamma_R^{(2)}(0) = \Gamma_B^{(2)}(q)|_{q^2=0} Z_\phi = \left[m_B^2 + \Sigma_B(0)\right] Z_\phi = m^2 \tag{9.87}$$

The wave function renormalization is fixed by making the slope of $\Gamma_R^{(2)}$ equal to unity at the origin [note that $\Sigma_R(q)$ starts out with q^4 because of the double substraction in (9.55)]. Hence

$$\left.\frac{\partial}{\partial q^2} \Gamma_R^{(2)}(q^2)\right|_{q^2=0} = \left.\frac{\partial}{\partial q^2} \Gamma_B^{(2)}(q)\right|_{q^2=0} Z_\phi = \left[1 + \frac{\partial}{\partial q^2} \Sigma^B(0)\right] Z_\phi = 1. \tag{9.88}$$

Finally, the renormalized coupling is given by

$$\Gamma_R^{(4)}(0) = g_B \Gamma_B^{(4)}(0) Z_\phi^2 = g. \tag{9.89}$$

This leads to the three equations:

$$
\begin{aligned}
m_R^2 &= \left[m_B^2 + \frac{g_B}{2} D_1^B - \frac{g_B^2}{4} D_2^B D_1^B - \frac{g_B^2}{6} D_3^B(0)\right] Z_\phi, \\
g_R &= \left[g_B - \frac{3}{2} g_B^2 I^B(0) + \frac{3}{4} g_B^3 I^{B^2}(0) + \frac{3}{2} g_B^3 I_3^B(0) D_1^B + 3 g_B^3 I_4^B(0)\right] Z_\phi^2, && (9.90)\\
1 &= \left[1 - \frac{g_B^2}{6} D_3^{B'}(0)\right] Z_\phi. && (9.91)
\end{aligned}
$$

We now solve these three equations for g_B, m_B in terms of g, m by inserting on the right-hand sides the power series expansions

$$\begin{aligned} g_B &= \sum_{n=1}^{\infty} a_n g^n, \\ m_B^2 &= m_R^2 \sum_{1}^{\infty} b_n g^n, \\ Z_\phi &= 1 + \sum_{n=1}^{\infty} c_n g^n, \end{aligned} \tag{9.92}$$

and determining the coefficients a_n, b_n, c_n order by order in g. To first order in g there are only few terms, and we can proceed less systematically in two steps. First, we forget for a moment (9.91), set $Z_\phi = 1$, and call the masses and coupling constants emerging from (9.90) and (9.90) $\bar{m}^2$ and $\bar{g}$, respectively. Inverting (9.90) we have

$$m_B^2 = \bar{m}^2 - \frac{g_B}{2} \bar{D}_1 + \mathcal{O}(g_B^2), \tag{9.93}$$

where $\bar{D}_1$ is the same expression as D_1, except with m^2 replaced by $\bar{m}^2$. Inserting this into (9.90), we may replace m_B by m_R in all functions I, D. The only exception is $I^B(0)$ where a first-order correction (9.93) must be taken into account, leading to

$$I^B(0) = I^R(0) + g_B I_3^R(0) D_1^R + \mathcal{O}(g_B^2). \tag{9.94}$$

In this way we have accounted for all terms of order g_B^2, and Eq. (9.90) yields

$$\bar{g} = g_B - \frac{3}{2} g_B^2 \bar{I}(0) + \frac{3}{4} g_B^3 \bar{I}(0)^2 + 3 g_B^3 \bar{I}_4(0). \tag{9.95}$$

Inverting this gives

$$g_B = \bar{g} + \frac{3}{2} \bar{g}^2 \bar{I}(0) + \frac{15}{4} \bar{g}^3 \bar{I}(0)^2 - 3 \bar{g}^3 \bar{I}_4(0). \tag{9.96}$$

Now we observe that with (9.93), the term D_1^B in (9.90) can be reexpanded as

$$D_1^B = \bar{D}_1 + \frac{g_B}{2} \bar{D}_1 \bar{D}_2, \tag{9.97}$$

so that (9.90) takes the form

$$\bar{m}^2 = m_B^2 + \frac{g_B}{2} \bar{D}_1(0) - \frac{g_B^2}{6} \bar{D}_3(0). \tag{9.98}$$

Together with (20.32), this yields

$$m_B^2 = \bar{m}^2 - \frac{g_1}{2} \bar{D}_1 - \frac{3}{4} \bar{g}^2 \bar{I}(0) \bar{D}_1 + \frac{1}{6} \bar{g}^2 \bar{D}_3(0). \tag{9.99}$$

On the right-hand sides of this and (20.32) we recognize precisely the counterterms (9.74) calculated with $\bar{m}$, $\bar{g}$ instead of m, g. This is in agreement with the multiplicative renormalization laws (9.79), since we assumed for the moment $Z_\phi = 1$ or $c^\phi = 0$, in which case Eqs. (9.78)–(9.80) take the form

$$\begin{aligned} \phi_B &= \phi_1, \\ m_B^2 &= \bar{m}^2 Z_m, \\ g_B &= \bar{g} Z_g. \end{aligned} \tag{9.100}$$

Let us finally include the effect of Z_ϕ and go from $\bar{m}$, $\bar{g}$ to m, g. Since

$$Z^\phi = \left[1 - \frac{g^2}{6} D_3^{R\prime}(0)\right]^{-1} \tag{9.101}$$

is of second order in g_B, we have to this order

$$Z^\phi = 1 + \frac{\bar{g}^2}{6} \bar{D}_3{}'(0) + \ldots = 1 + c_R^\phi + \ldots . \tag{9.102}$$

We now determine m, g from

$$\bar{m}^2(1 + c_1^{m^2}) = m_R^2(1 + c_R^{m^2})(1 + c_R^\phi)^{-1}, \tag{9.103}$$

$$\bar{g}(1 + c_1^g) = g_R(1 + c_R^g)(1 + c_R^\phi)^{-2}. \tag{9.104}$$

The first of these equations shows that m^2 and m_1^2 differ by a term quadratic in g_1^2:

$$m_1^2 = m_R^2 \left[1 - \frac{g_1^2}{6} D_3^1(0) + \ldots\right], \tag{9.105}$$

which can be written as

$$m_1^2 = m_R^2 \left[1 - \frac{g_R^2}{6} D_3^{R\prime}(0) + \ldots\right], \tag{9.106}$$

without changing terms of order g^2. Inserting this into (9.99) yields

$$m_B^2 = m_R^2 - \frac{g_R}{2} D_1^R - \frac{3}{4} g_R^2 I^R(0) D_1^R + \frac{1}{6} g_R^2 D_3^R(0) - m_R^2 \frac{g_R^2}{6} D_3^{R\prime}(0). \tag{9.107}$$

Inserting (9.106) into (20.32), we can replace m_1 by m without mistake up to order g_1^3. But then we see from (9.104) that

$$g_1 = g_R \left[1 - \frac{g_R^2}{3} D_3^{R\prime}(0) + \ldots\right], \tag{9.108}$$

i.e., g_1 differs from g_R only by a correction term of second order. Combined with (9.95), this implies

$$g_B = g_R + \frac{3}{2} g_R^2 I^R(0) + \frac{15}{4} g_R^3 I^R(0)^2 - 3 g_R^3 I_4^R(0) - \frac{g_R^3}{3} D_3^{R\prime}(0). \tag{9.109}$$

Again we find precisely the same counterterms as in (9.76). This completes the renormalization program with the bare quantities as a starting point and applying the normalization conditions (9.90), (9.90), (9.91).

As we mentioned before, the finite values g_R, m_R do not correspond to what we would experimentally identify as the physical coupling constants of the particles. The mass would be defined by the pole of $G^{(2)}$, i. e. by the zero of $\Gamma^{(2)}$

$$\Gamma^{(2)}(q)\Big|_{q^2=-m^2_{\text{ph}}} = 0 \tag{9.110}$$

and the physical coupling by

$$\Gamma^{(4)}(q_i)\Big|_{\text{MS}} = g_{\text{ph}} \tag{9.111}$$

where the subscript MS denotes the point where all legs are on the mass shell, i. e. correspond to physical particles

$$\begin{aligned} q_i^2 &= m^2 \\ q_i q_j &= \frac{m^2}{3}\left(4\delta_{ij}-1\right) \end{aligned} \tag{9.112}$$

such that $(q_i+q_j)^2 = \frac{4}{3}m^2$.

The wave function normalization at the physical pole would be set equal to unity by

$$\frac{\partial\Gamma_R(q)}{\partial q^2}\Bigg|_{q^2=-m^2_{\text{ph}}} = 1. \tag{9.113}$$

Then all vertex functions would be directly expressed in terms of these physical values. The difference between these and the previous m, g are calculable in terms of a multiplicative renormalization whose factors are power series in g with only *finite* coefficients.

9.5 Dimensional Regularization of Integrals

There is another method for making Feynman integrals finite with a specific control over the divergences. It has the advantage of not needing the specification of a subtraction point in momentum space. Moreover, in field theories other than ϕ^4 which contain massless particles and are gauge invariant it preserves all symmetry relations between the Green functions which are generally destroyed by the previous regularization methods (in particular the so-called *Ward identities*). Instead of employing a cutoff it is possible to analytically continue the Feynman integrals to a continuous spacetime dimension in the neighborhood of the physical dimension $D=4$.

Starting point of this method is the observation that a Feynman propagator can be written as

$$\frac{1}{k^2+2kq+m^2} = \int_0^\infty d\tau e^{-\tau\left(k^2+2kq+m^2\right)}, \quad k^2+2kq+m^2>0. \tag{9.114}$$

This can be generalized to

$$\frac{1}{\left(k^2+2kq+m^2\right)^\nu}=\frac{1}{\Gamma(\nu)}\int_0^\infty\frac{d\tau}{\tau}\tau^\nu e^{-\tau\left(k^2+2kq+m^2\right)},\quad k^2+2kq+m^2>0, \tag{9.115}$$

which is valid for all real $\nu>0$.

Consider now the typical Feynman integral

$$\int d\!\!\!{}^-{}^D k\frac{1}{\left(k^2+2kq+m^2\right)^\nu}=\frac{1}{\Gamma(\nu)}\int_0^\infty\frac{d\tau}{\tau}\tau^\nu\int d\!\!\!{}^-{}^D k e^{-\tau\left(k^2+2kq+m^2\right)}. \tag{9.116}$$

where $D=1,2,3,\dots$, and

$$d\!\!\!{}^-{}^D k\equiv\frac{d^Dk}{(2\pi)^D}. \tag{9.117}$$

The D-dimensional momentum integral on the right-hand side is trivial:

$$\int d\!\!\!{}^-{}^D k\, e^{-\tau\left(k^2+2kq+m^2\right)}=\frac{1}{(2\pi)^D}\left(\frac{\pi}{\tau}\right)^{D/2}e^{-\tau\left(m^2-q^2\right)}, \tag{9.118}$$

since after a quadratic completion of the exponential it factorizes into D products of Gaussian integrals. This equation forms the basis for the definition of Feynman diagrams in a continuous number of spacetime dimensions. We simply define the left-hand side of (9.116), (9.118) for all complex D via the analytic continuation of the right-hand side of (9.118). Then we can perform in (9.116) the integral over τ using the formula

$$\int_0^\infty d\tau\tau^{\nu-D/2-1}e^{-\tau a}=\Gamma\left(\nu-D/2\right)\frac{1}{a^{\nu-D/2}},\qquad a>0. \tag{9.119}$$

Note that although the integral on the left-hand side exists only for $D<2\nu$, the right-hand side provides an analytic continuation to larger $D>2\nu$ if one goes around the singularities at $D=2\nu,2\nu+2,2\nu+4\dots$. The extension can be made explicit by rewriting the left-hand side as follows:

$$\int_0^\infty d\tau\tau^{\nu-D/2-1}e^{-\tau a}=\int_c^\infty d\tau\tau^{\nu-D/2-1}e^{-\tau a}+\int_0^c d\tau\tau^{\nu-D/2-1}(e^{-\tau a}-1)+\frac{c^{\nu-D/2}}{\nu-D/2}, \tag{9.120}$$

with some parameter $c>0$ on which the right-hand side does not depend. In contrast to the original integral, the right-hand side is now defined for $2\nu<D<2\nu+2$. In the limit $c\to0$ we fall back onto the original integral. For $2\nu<D<2\nu+2$, however, we can take the limit $c\to\infty$ and we obtain the continuation rule

$$\int_0^\infty d\tau\tau^{\nu-D/2-1}e^{-\tau a}\equiv\int_0^\infty d\tau\tau^{\nu-D/2-1}(e^{-\tau a}-1). \tag{9.121}$$

If D approaches 2ν from above, the decomposition (9.120) for $c > 0$ shows that the integral is singular like $1/(\nu - D/2)$. The precise result is

$$\int \bar{d}^D k \frac{1}{\left(k^2 + 2kq + m^2\right)^\nu} = \frac{1}{(2\pi)^D} \frac{\pi^{D/2}}{(m^2 - q^2)^{\nu - D/2}} \frac{\Gamma\left(\nu - D/2\right)}{\Gamma(\nu)}. \tag{9.122}$$

This equation is valid by analytic continuation in the entire complex D-plane except at the singularities $D = 2\nu, 2\nu + 2, 2\nu + 4, \ldots$ of the Gamma function.

The analytic continuation has a peculiar feature which is worth emphasizing since it has important applications in massless theories (in particular gauge theories): For all D which do not lie at the above singular points the limit $\nu \to 0$ is well-defined and gives

$$\int \bar{d}^D k = 0. \tag{9.123}$$

If one defines the integral at the singular points by analytic continuation from the neighborhood it vanishes identically for all D. Let us split (9.123) into an angular and radial integral, and rewrite it as

$$S_D \int dk\, k^{D-1} = 0, \tag{9.124}$$

where S_D is the surface of a sphere in D dimensions ($S_1 = 2,\ S_2 = 2\pi,\ S_3 = 4\pi,\ S_4 = 2\pi^2, \ldots$).

$$S_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}. \tag{9.125}$$

Since D is arbitrary, we see the vanishing of the general homogeneous integral

$$\frac{S_D}{(2\pi)^D} \int dk\, k^{D-1} k^{-2\nu} = 0, \tag{9.126}$$

which holds for all ν. Written differently, we have

$$\int \bar{d}^D k\, k^{-2\nu} = 0. \tag{9.127}$$

This is known as *Veltman's integral rule*.

If we take $q = 0$ and the limit $m \to 0$ directly in the integral formula (9.122) for $\nu \neq 0$, the same result is obviously true only for $D > 2\nu$ where the integral is proportional to $m^{D-2\nu}$. Dor $D > 2\nu$, the limiting integral $\int \bar{d}^D k\, k^{-2\nu}$ is regular at $k = 0$. How that integral can be continued In 9.126 we show how that integral can be continued to the singular regime $D \leq 2\nu$.

The integral (9.126) contains a prefactor which will occur in all Feynman integrals. It will be useful call it, in analogy with the measure of integration (9.117), the *reduced surface* of a unit sphere ($\bar{S}_1 = 1/\pi,\ \bar{S}_2 = 1/2\pi,\ \bar{S}_3 = 1/2\pi^2,\ \bar{S}_4 = 1/8\pi^2, \ldots$).

$$\bar{S}_D \equiv \frac{S_D}{(2\pi)^D} = \frac{1}{(2\pi)^D}\frac{2\pi^{D/2}}{\Gamma(D/2)} = \frac{1}{(4\pi)^{D/2}}\frac{2}{\Gamma(D/2)}. \tag{9.128}$$

In the perturbation series to be derived, the factor $\bar{S}_D$ will accompany each power of the coupling constant and may be absorbed into it [see (9.212)].

With the reduced surface of a sphere, the Feynman integral (9.122) may be rewritten as

$$\int \bar{d}^D k \frac{1}{(k^2+2kq+m^2)^\nu} = \bar{S}_D \frac{1}{2}\frac{\Gamma(D/2)\Gamma(\nu-D/2)}{\Gamma(\nu)}\frac{1}{(m^2-q^2)^{\nu-D/2}}. \tag{9.129}$$

This integral may be used to derive several other Feynman integrals, by forming successive derivatives with respect to the momentum four-vector k, and find the formulas

$$\int \bar{d}^D k \frac{k_\mu}{(k^2+2kq+m^2)^\nu} = \frac{\Gamma(D/2)\Gamma(\nu-D/2)}{2\Gamma(\nu)}\frac{1}{(m^2-q^2)^{\nu-D/2}}(-q_\mu), \tag{9.130}$$

$$\begin{aligned} \int \bar{d}^D k \frac{k_\mu k_\nu}{(k^2+2kq+m^2)^\nu} &= \frac{\Gamma(D/2)}{2\Gamma(\nu)}\frac{1}{(m^2-q^2)^{\nu-D/2}}, \\ &\times\left[\Gamma(\nu-D/2)\,q_\mu q_\nu + \Gamma(\nu-1-D/2)\,\frac{1}{2}\delta_{\mu\nu}(m^2-q^2)\right], \end{aligned} \tag{9.131}$$

$$\begin{aligned} \int \bar{d}^D k \frac{k_\mu k_\nu k_\lambda}{(k^2+2kq+m^2)^\nu} &= \frac{\Gamma(D/2)}{2\Gamma(\nu)}\frac{1}{(m^2-q^2)^{\nu-D/2}} \\ \times\left[-\Gamma(\nu-D/2)\,k_\mu k_\nu k_\lambda - \Gamma(\nu-1-D/2)\,\frac{1}{2}(\delta_{\mu\nu}k_\lambda + \delta_{\mu\lambda}k_\nu + \delta_{\nu\lambda}k_\mu)(m^2-q^2)\right]. \end{aligned} \tag{9.132}$$

By expanding (9.122) up to order $\mathcal{O}(\nu)$ and comparing the coefficients of ν we find a further important integral

$$\int \bar{d}^D k \log(k^2+2kq+m^2) = \bar{S}_D \frac{1}{D}\Gamma(D/2)\Gamma(1-D/2)\ (m^2-q^2)^{D/2}, \tag{9.133}$$

Strictly speaking, the logarithm on the left-hand side does not make sense since its argument has the dimension of a square mass. It should therefore always be written as $\log[(k^2+2kq+m^2)/\mu^2]$ with some auxiliary mass μ. If m if $m \neq 0$, the auxiliary mass μ can, of course, be set equal to m. In dimensional regularization, however, this proper way of writing the logartihm does not change the integral at all, since it merely amounts to adding an integral over a constant, and this vanishes by Veltman's rule (9.127).

Note that when forming the trace of (9.131) in the indices $\mu\nu$, we obtain the same result as in a direct calculation with k^2 in the numerator, the trivial trace formula

$$\delta_{\mu\mu} \equiv D, \tag{9.134}$$

which is initially valid only for integer D, is comtinued to arbitrary continuous dimensions D.

The above integrals are finite except for certain integer values of D. By setting $D = 4-\varepsilon$ with some small number ε, all integrals can be made finite without a cutoff Λ. The finiteness is achieved by a particular analytic continuation of the spacetime dimension away from the integer values of D. For this reason, the above way of making Feynman integrals finite is called the method of dimensional regularization, or of *analytic regularization*.

Let us now study the Feynman integrals occurring in Eqs. (9.26) (9.31) for real D near the physical dimension $D = 4$. The first integral is (9.26):

$$1) \quad D_1 = \int d^D k \frac{1}{k^2+m^2} = \bar{S}_D \frac{1}{2} \Gamma(D/2)\Gamma(1-D/2)(m^2)^{-1+D/2}. \tag{9.135}$$

The divergence of this integral manifests itself in the pole of the Gamma function at the physical dimension $D = 4$. In the neighborhood of this dimension we set

$$D \equiv 4-\varepsilon \tag{9.136}$$

and express the integral in terms of ε. The singularity at small ε may be isolated by using the expansions

$$\begin{aligned} \Gamma(x) &= \frac{1}{x}\Gamma(1+x), \\ \Gamma(1+x)\Gamma(1-x) = \frac{\pi x}{\sin \pi x} &= 1 + \frac{\pi^2}{6}x^2 + \dots . \end{aligned} \tag{9.137}$$

Note that the second relation has only quadratic correction terms ε^2. There is a useful generalization of this,

$$\frac{\prod_n \Gamma(1+a_n\varepsilon)}{\prod_m \Gamma\left(1+a'_m\varepsilon\right)} = 1 + \mathcal{O}\left(\varepsilon^2\right) \tag{9.138}$$

if

$$\sum_n a_n - \sum_m a'_m = 0. \tag{9.139}$$

This relation ensures the cancelation of all terms proportional to ε when expanding $\Gamma(1+a\varepsilon) = 1 - \gamma\varepsilon + \mathcal{O}\left(\varepsilon^2\right)$. With (9.137) we have

$$\begin{aligned} \Gamma(D/2)\Gamma(1-D/2) &= \Gamma\left(2-\frac{\varepsilon}{2}\right)\Gamma\left(-1+\frac{\varepsilon}{2}\right) = -\frac{2}{\varepsilon}\Gamma\left(1-\frac{\varepsilon}{2}\right)\Gamma\left(1+\frac{\varepsilon}{2}\right) \\ &= -\frac{2}{\varepsilon} + \mathcal{O}(\varepsilon) \end{aligned} \tag{9.140}$$

and therefore

$$D_1 = \bar{S}_D m^2 \cdot (m^2)^{-\varepsilon/2}\left[-\frac{1}{\varepsilon} + \mathcal{O}(\varepsilon)\right]. \tag{9.141}$$

This expression has a mass dimension $(m^2)^{1-\varepsilon/2}$ and a singularity proportional to $1/\varepsilon$. It may be separated into a singular and a regular expression

$$D_1 \equiv D_1^{\rm sg} + D_1^{\rm reg}, \tag{9.142}$$

with

$$D_1^{\rm sg} \equiv -\bar{S}_D (m^2)^{1-\varepsilon/2} \frac{1}{\varepsilon}. \tag{9.143}$$

The singular is not uniquely defined. It may be modified by an arbitrary regular term. For instance, we may introduce an arbitrary fixed mass scale μ and choose as a singular part

$$D_1^{\rm sg} \equiv -\bar{S}_D m^2 \left(\mu^2\right)^{-\varepsilon/2} \frac{1}{\varepsilon}. \tag{9.144}$$

The two choices differ by a regular term $\frac{1}{2}\bar{S}_D \log(m^2/\mu^2)$. The latter choice has the form m^2 multiplied function which is independent of the mass m. We shall see below that this property persists to higher orders in perturbation. This property will later be of great advantage in studying the theory in the limit $m \to 0$. The scale parameter μ is unavoidable when taking this limit.

It also will simplify the develompent of the so-called renormalization group in Chapter 21, which governs critical phenomena observed in second-order phase transitions. [2] By virtue of μ it will be possible to

By comparing the singular term (9.144) with the previous cutoff divergence which was

$$D_1 = \frac{1}{(4\pi)^2}\Lambda^2 \tag{9.145}$$

we realize that the quantity $1/\varepsilon$ plays the same role as before Λ^2/m^2.

A similar subtraction procedure is applied to the other Fenyman integrals. Consider (9.27):

$$2) \quad D_2 = \int \bar{d}^D k \frac{1}{(k^2+m^2)^2} = \bar{S}_D \frac{1}{2} \frac{\Gamma(D/2)\Gamma(2-D/2)}{\Gamma(2)} (m^2)^{D/2-2}. \tag{9.146}$$

Now

$$\Gamma(D/2)\Gamma(2-D/2) = (1-D/2)\left[-\frac{2}{\varepsilon} + \mathcal{O}(\varepsilon)\right] \tag{9.147}$$

$$= \frac{2}{\varepsilon} - 1 + \mathcal{O}(\varepsilon) \tag{9.148}$$

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[2] H. Kleinert, J. Neu, V. Schulte-Frohlinde, K.G. Chetyrkin, and S.A. Larin, *Five-Loop Renormalization Group Functions of O(n)-symmetric φ^4-Theory and ε-Expansions of Critical Exponents up to ε^5*, Phys. Lett. **B272**, 39 (1991); H. Kleinert and V. Schulte-Frohlinde, Exact Five-Loop Renormalization Group Functions of ϕ^4-Theory with O(N)-Symmetric and Cubic Interactions. Critical Exponents up to ε^5, Phys. Lett. **B 342**, 284 (1995); H. Kleinert and V. Schulte-Frohlinde *Critical Phenomena in Φ^4-Theory*, (in preparation).

so that

$$D_2 = \bar{S}_D (m^2)^{-\varepsilon/2}\left[\frac{1}{\varepsilon} - \frac{1}{2} + \mathcal{O}(\varepsilon)\right] \equiv D_2^{\rm sg} + D_2^{\rm reg}. \tag{9.149}$$

Here we choose as a singular part the expression

$$D_2^{\rm sg} \equiv \bar{S}_D \mu^{-\varepsilon}\frac{1}{\varepsilon}. \tag{9.150}$$

The mass parameter μ ensures the correct dimension of both singular and regular terms, and makes the singular term independent of the mass m. This is again useful for a study of the theory in the massless limit. Another advantage of introducing the mass parameter μ is that the singular parts (9.144) and (9.150) is that $D_2^{\rm sg}$ is related to the singular part $D_1^{\rm sg}$ by derivative $-\partial/\partial m^2$:

$$D_2^{\rm sg} = \frac{\partial}{\partial m^2} D_1^{\rm sg}. \tag{9.151}$$

The pole term $1/\varepsilon$ replaces a logarithmic divergence that woul appear in a cutoff regularization. Since also the quadratic divergence in D_1 had a $1/\varepsilon$ pole, one may wonder how the singularities in ε can reflect the difference between quadratic and logarithmic divergence in the cutoff method: Comparison with D_1 shows that while D_2 has its lowest singularity at $D = 4$, i.e., its highest singularity at $\varepsilon = 0$, D_1 has it at $D = 2$, i.e., the highest singularity lies at $\varepsilon = 2$.

Consider now the Feynman integral (9.29):

$$3) \qquad I(q) = \int \bar{d}^D k \frac{1}{\left(k^2 + m^2\right)\left[(k-q)^2 + m^2\right]}. \tag{9.152}$$

Here we use Feynman's formula

$$\frac{1}{AB} = \int_0^1 dx \frac{1}{[Ax + B(1-x)]^2} = \int_0^1 dx \frac{1}{[A(1-x) + Bx]^2} \tag{9.153}$$

which follows from the trivial relation

$$\frac{1}{AB} = \frac{1}{B-A}\left(\frac{1}{A} - \frac{1}{B}\right) = \frac{1}{B-A}\int_A^B dz \frac{1}{z^2}. \tag{9.154}$$

For n denominators, Feynman's formula reads[3]

$$\frac{1}{A_i \cdots A_n} = (n-1)! \int_0^1 \int_0^1 dx_1 \ldots dx_n \frac{\delta\left(\sum_{i=1}^n x_i - 1\right)}{\left(A_1 x_1 + \ldots + A_n x_n\right)^n}, \tag{9.155}$$

as can be proved by induction. By differentiating both sides α_i times with respect to A_i, one finds more generally

$$\frac{1}{A_1^{\alpha_1} \cdots A_n^{\alpha_n}} = \frac{\Gamma\left(\sum_{i=1}^n \alpha_i\right)}{\prod^n{}_{i=1}\Gamma(\alpha_i)} \prod_{i=1}^n \int_0^1 dx_i \frac{\prod_{i=1}^n x_i^{\alpha_i - 1}\delta\left(\sum_{i=1}^n x_i - 1\right)}{\left[\sum_{i=1}^n x_i A_i\right]^{\sum_{i=1}^n \alpha_i}}. \tag{9.156}$$

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[3] For a proof of this formula see Vol. I of E. Goursat and E.R. Hedrick, *A Course in Mathematical Analysis*, Ginn and Co., Boston, 1904.

By analytic continuation, this formula remains valid for complex values of α_i.

Using (9.153) and the substitution $z = Ax + B(1-x)$, we rewrite (9.152) as

$$\begin{aligned} I(q) &= \int_0^1 dx \int d^D k \frac{1}{\left\{\left(k^2+m^2\right)(1-x) + \left[(k+q)^2+m^2\right]x\right\}^2} \\ &= \int_0^1 dx \int d^D k \frac{1}{\left[k^2+2kqx+q^2x+m^2\right]^2}. \end{aligned} \tag{9.157}$$

The momentum integration gives

$$I(q) = S_D \frac{1}{2}\Gamma(D/2)\Gamma(2-D/2)\int_0^1 dx \frac{1}{\left[q^2x(1-x)+m^2\right]^{2-D/2}}. \tag{9.158}$$

Going over to the variable ε, we rewrite this as

$$I(q) = S_D \frac{1}{2}\Gamma(2-\varepsilon/2)\,\Gamma(\varepsilon/2)\,\mu^{-\varepsilon}\int_0^1 dx \frac{(\mu^2)^{\varepsilon/2}}{\left[q^2x(1-x)+m^2\right]^{\varepsilon/2}}. \tag{9.159}$$

We have used once more the mass parameter μ to make the integral dimensionless. The integral is regular at $\varepsilon = 1$. A singularity comes only from the prefactor, which possesses a $1/\varepsilon$ -behavior to be extracted with the help of formula (9.137):

$$\begin{aligned} \Gamma(2-\varepsilon/2)\Gamma(\varepsilon/2) &= \left(1-\frac{\varepsilon}{2}\right)\frac{2}{\varepsilon}\Gamma\left(1-\frac{\varepsilon}{2}\right)\Gamma\left(1+\frac{\varepsilon}{2}\right) \\ &= \frac{2}{\varepsilon} - 1 + \mathcal{O}(\varepsilon). \end{aligned} \tag{9.160}$$

Hence we obtain

$$I(q) = S_D \frac{1}{\varepsilon}\left(1-\frac{\varepsilon}{2}\right)\mu^{-\varepsilon}\left(\frac{\mu^2}{q^2}\right)^{\varepsilon/2} J_\varepsilon^m(q), \tag{9.161}$$

with the integral

$$J_\varepsilon^m(q) = \int_0^1 dx \left[x(1-x) + \frac{m^2}{q^2}\right]^{-\varepsilon/2}. \tag{9.162}$$

For $m = 0$, the integral can immediately be done:

$$J_\varepsilon^m(q) \equiv J_\varepsilon^0 = \int_0^1 x^a (1-x)^b = \frac{\Gamma(a+1)\Gamma(b+1)}{\Gamma(a+b+2)} \tag{9.163}$$

with

$$J_\varepsilon^0 = \frac{\Gamma^2(1-\varepsilon/2)}{\Gamma(2-\varepsilon)} = 1 + \varepsilon + \mathcal{O}(\varepsilon^2). \tag{9.164}$$

We may therefore expand

$$I(q) = S_D \left(\frac{1}{\varepsilon} + \frac{1}{2}\right) \mu^{-\varepsilon} \left(\frac{\mu^2}{q^2}\right)^{\varepsilon/2} + \mathcal{O}(\varepsilon). \tag{9.165}$$

The residue at the pole is independent of q, as a manifestation of the renormalizability of the theory. For $m \neq 0$, we can expand (9.162) in powers of m and find the same pole term in ε. This property is a special feature of this regularization procedure.

We now choose the singular part

$$I^{\rm sg} \equiv S_D \frac{\mu^{-\varepsilon}}{\varepsilon}, \tag{9.166}$$

to form the subtracted Feynman integral

$$I^{\rm reg}(q) = I(q) - I^{\rm sg}, \tag{9.167}$$

which is smooth in the limit $\varepsilon \to 0$. As before, we have included the factor $\mu^{-\varepsilon}$ in (9.166) for dimensional reasons.

For $m \neq 0$, we expand $J_\varepsilon^m(q)$ in powers of ε and find an additional factor

$$1 - \frac{\varepsilon}{2}\left[L^m(q) - L^0\right], \tag{9.168}$$

where

$$\begin{aligned} L^m(q) &= \int_0^1 dx \log\left[x(1-x) + \frac{m^2}{q^2}\right] \\ &= -2 + \log\frac{m^2}{q^2} + \frac{\sqrt{q^2+4m^2}}{\sqrt{q^2}} \log\frac{\sqrt{q^2+4m^2}+\sqrt{q^2}}{\sqrt{q^2+4m^2}-\sqrt{q^2}}. \end{aligned} \tag{9.169}$$

This can also be written as

$$L^m(q) = -2 + \log\frac{m^2}{q^2} + 2\theta \coth\theta. \tag{9.170}$$

with

$$\sinh^2\theta = \frac{q^2}{4m^2} \tag{9.171}$$

or

$$\theta = \operatorname{atanh}\frac{\sqrt{q^2}}{\sqrt{q^2+4m^2}} = \frac{1}{2}\log\frac{\sqrt{q^2+4m^2}+\sqrt{q^2}}{\sqrt{q^2+4m^2}-\sqrt{q^2}}. \tag{9.172}$$

For $m = 0$, $L^0(q)$ becomes a constant: $L^0(q) \equiv L^0 = -2$.

Altogether, we obtain for any mass m:

$$I(q) = S_D \mu^{-\varepsilon} \left[\frac{1}{\varepsilon} - \frac{1}{2} - \frac{1}{2} L^m(q) - \frac{1}{2} \log \frac{q^2}{\mu^2}\right] + \mathcal{O}(\varepsilon). \qquad (9.173)$$

The singularity is the same as in the $m = 0$ -expression (9.165), so that the subtraction (9.167) regularizes the integral for all m. Note the subtraction constant of $D_2(q)$ is the same as that of $I(q)$:

$$I^{\rm sg} = D_2^{\rm sg}, \qquad (9.174)$$

which is obvious from the definitions (9.27) and (9.29) and the mass and momentum independence of the singular parts.

The result (9.173) can now be applied to the calculation of the Feynman integral (9.28):

$$4) \quad D_3(q) = \int d^D k_1 d^D k_2 \frac{1}{(k_1^2 + m^2)(k_2^2 + m^2)} \frac{1}{\left[(q + k_1 + k_2)^2 + m^2\right]}. \qquad (9.175)$$

In $D = 4$ dimensions, this integral contains 8 momentum integrations and only 6 powers of momenta in the denominator, so that it diverges formally like Λ^2. Before applying Feynman's formula (9.156), we decrease the degree of divergence by a partial integration trick due to 't Hooft and Veltman.[4]

Partial differentiation with respect to the momentum variables satisfies the trivial identity:

$$\frac{\partial k^\mu}{\partial k^\nu} = \delta^\mu{}_\nu. \qquad (9.176)$$

Contracting the indices in D dimensions as in (9.134) gives

$$\frac{\partial k^\mu}{\partial k^\mu} = D. \qquad (9.177)$$

Thus we may insert into the integral (9.175) the trivial identity

$$1 = \frac{1}{2D} \left(\frac{\partial k_1^\mu}{\partial k_1^\mu} + \frac{\partial k_2^\mu}{\partial k_2^\mu}\right). \qquad (9.178)$$

After an integration by parts neglecting surface terms, we may write

$$\begin{aligned} D_3(q) &= -\frac{1}{2D} \int d^D k_1 d^D k_2 \left(k_1^\mu \frac{\partial}{\partial k_1^\mu} + k_2^\mu \frac{\partial}{\partial k_2^\mu}\right) \\ &\quad \times \frac{1}{(k_1^2 + m^2)(k_2^2 + m^2)} \frac{1}{\left[(q + k_1 + k_2)^2 + m^2\right]}. \end{aligned}$$

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[4] G. 't Hooft and H. Veltman, Nucl. Phys. B *44*, 189 (1972). See also Curtright and Ghandour, Ann. Phys. *106*, 209 (1977).

Performing the differentiations leads to the following decomposition of $D_3(q)$:

$$\begin{aligned} D_3(q) &= -\frac{1}{D-3}\int \bar{d}^D k_1 \bar{d}^D k_2 \frac{3m^2 + q(q+k_1+k_2)}{(k_1^2+m^2)(k_2^2+m^2)\left[(q+k_1+k_2)^2+m^2\right]^3} \\ &= -\frac{1}{D-3}\left[3m^2 A(q) + B(q)\right]. \end{aligned} \tag{9.179}$$

where

$$A(q) = \int \bar{d}^D k_1 \bar{d}^D k_2 \frac{1}{(k_1^2+m^2)^2(k_2^2+m^2)\left[(q+k_1+k_2)^2+m^2\right]}, \tag{9.180}$$

and

$$B(q) = \int \bar{d}^D k_1 \bar{d}^D k_2 \frac{q(q+k_1+k_2)}{(k_1^2+m^2)(k_2^2+m^2)\left[(q+k_1+k_2)^2+m^2\right]^2}. \tag{9.181}$$

The first integral is only logarithmically divergent. the second linearly. These integrals are now evaluated with the help of Feynman's formula (9.153). We begin with $A(q)$, which can obviously be rewritten as

$$\begin{aligned} A(q) &= \int \bar{d}^D k_1 \frac{1}{(k_1^2+m^2)^2} I(k_1+q) \\ &= \bar{S}_D \frac{1}{2}\Gamma(D/2)\Gamma(2-D/2) \\ &\quad\times \int_0^1 dx \int \bar{d}^D k \frac{1}{(k^2+m^2)^2} \frac{1}{\left[(q+k)^2 x(1-x)+m^2\right]^{2-D/2}}. \end{aligned} \tag{9.182}$$

We remove a factor $[x(1-x)]^{2-D/2}$ from the denominator and apply to the remaining integrand the generalized Feynman formula (9.156) in the form

$$\frac{1}{A^\alpha}\frac{1}{B^\beta} = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\int_0^1 dy \frac{y^{\alpha-1}(1-y)^{\beta-1}}{[Ay+B(1-y)]^{\alpha+\beta}}. \tag{9.183}$$

This leads to

$$A(q) = \bar{S}_D \frac{1}{2}\Gamma(D/2)\Gamma(2-D/2)\frac{\Gamma(4-D/2)}{\Gamma(2)\Gamma(2-D/2)} \tag{9.184}$$

$$\times \int_0^1 dx\, [x(1-x)]^{D/2-2} \int_0^1 dy \int \bar{d}^D k \frac{y(1-y)^{1-D/2}}{f^{4-D/2}(q;k,x,y)} \tag{9.185}$$

with

$$\begin{aligned} f(q;k,x,y) &= y(k^2+m^2) + (1-y)\left[(q+k)^2 + \frac{m^2}{x(1-x)}\right] \\ &= k^2 + (2kq+q^2)(1-y) + m^2\left[y + \frac{1-y}{x(1-x)}\right]. \end{aligned} \tag{9.186}$$

By integrating this over $\bar{d}^D k$, we obtain

$$\begin{aligned} A(q) &= \bar{S}_D^2 \frac{1}{2}\Gamma(D/2)\Gamma\left(2-D/2\right)\frac{\Gamma(4-D/2)}{\Gamma(2)\Gamma(2-D/2)} \\ &\times\frac{1}{2}\frac{\Gamma(D/2)\Gamma(4-D)}{\Gamma(4-D/2)}\int_0^1 dx\,[x(1-x)]^{D/2-2} \\ &\times\int_0^1 dy\,y\,(1-y)^{1-D/2}\left\{q^2 y(1-y)+m^2\left[y+\frac{1-y}{x(1-x)}\right]\right\}^{D-4}, \end{aligned} \tag{9.187}$$

which reads in terms of ε:

$$\begin{aligned} A(q) &= \bar{S}_D^2\frac{1}{4}\Gamma^2\left(2-\varepsilon/2\right)\Gamma(\varepsilon)(m^2)^{-\varepsilon}\int_0^1 dx\,[x(1-x)]^{-\varepsilon/2} \\ &\times\int_0^1 dy\,y\,(1-y)^{\varepsilon/2-1}\left\{\frac{q^2}{m^2}y(1-y)+\left[y+\frac{1-y}{x(1-x)}\right]\right\}^{-\varepsilon}. \end{aligned} \tag{9.188}$$

Defining the dimensionless expression in curly brackets as

$$F(q;x,y)\equiv\frac{q^2}{m^2}y(1-y)+\left[y+\frac{1-y}{x(1-x)}\right], \tag{9.189}$$

we expand

$$F^{-\varepsilon}(q;x,y)=1-\varepsilon\log F(q;x,y)+\mathcal{O}(\varepsilon^2). \tag{9.190}$$

The first term gives [via (9.163)]

$$\bar{S}_D^2\frac{1}{4}\Gamma^2\left(2-\varepsilon/2\right)\Gamma(\varepsilon)(m^2)^{-\varepsilon}\frac{\Gamma^2\left(1-\varepsilon/2\right)}{\Gamma(2-\varepsilon)}\frac{\Gamma(2)\Gamma\left(\varepsilon/2\right)}{\Gamma\left(2+\varepsilon/2\right)}. \tag{9.191}$$

This can be rewritten as

$$\bar{S}_D^2(m^2)^{-\varepsilon}\frac{1}{4}\left(1-\varepsilon/2\right)^2\frac{2}{\varepsilon^2}\frac{1}{1-\varepsilon}\frac{1}{1+\varepsilon/2}\frac{\Gamma^4(1-\varepsilon/2)\Gamma(1+\varepsilon)\Gamma(1+\varepsilon/2)}{\Gamma\left(1-\varepsilon\right)\Gamma\left(1+\varepsilon/2\right)}. \tag{9.192}$$

The ratio of Gamma-functions has the general form (9.138) with (9.139) and can be replaced by $1+\mathcal{O}(\varepsilon^2)$. Thus we obtain the first contribution to $A(q)$:

$$A(q)=\bar{S}_D^2\frac{(m^2)^{-\varepsilon}}{4\varepsilon}\left[\frac{2}{\varepsilon}-1+\mathcal{O}\left(\varepsilon\right)\right]. \tag{9.193}$$

We now turn to the second contribution in (9.188) due to the logarithm in the expansion (9.190). A singular term at $\varepsilon=0$ can only come from the end-point singulaity in the y-integral of (9.188) at $y=1$. Near that point, the logarithm goes to zero like

$$\log F(q;x,y)=\mathcal{O}(1-y), \tag{9.194}$$

so that the integral has no end-point singularity after all. Thus there is no further singular contribution to $A(q)$ in Eq. (9.225).

To complete the calculation of the pole terms in $D_3(q)$ we have to study the second integral $B(q)$ in Eq. (9.179). After applying again the Feynman formula twice we arrive at an expression of the type (9.188):

$$\begin{aligned} B(q) &= \bar{S}_D^2 \frac{1}{4}\Gamma^2\left(2-\varepsilon/2\right)\Gamma(\varepsilon)\, q^2 (m^2)^{-\varepsilon}\int_0^1 dx\,[x(1-x)]^{-\varepsilon/2} \\ &\quad \times \int_0^1 dy\, y\,(1-y)^{\varepsilon/2}\,[F(q;x,y)]^{-\varepsilon}\,. \end{aligned} \tag{9.195}$$

Here both the x- and the y-integrals are free of endpoint singularites and converge. At $\varepsilon = 0$, the integrals are equal to $1/2$. Thus we find the pole term of $B(q)$:

$$B(q) = \bar{S}_D^2 \frac{(m^2)^{-\varepsilon}}{4\varepsilon}\Gamma^2(2-\varepsilon/2)\Gamma(1+\varepsilon)\frac{q^2}{2} = \bar{S}_D^2 \frac{(m^2)^{-\varepsilon}}{4\varepsilon}\frac{q^2}{2}\left[1+\mathcal{O}(\varepsilon)\right]. \tag{9.196}$$

Inserting this and (9.193) into (9.179), we obtain for the singular part of $D_3(q)$:

$$D_3^{\rm sg}(q) = -\bar{S}_D^2 m^2 \mu^{-2\varepsilon}\frac{6}{4\varepsilon}\left[\frac{1}{\varepsilon} - 2\log\frac{m}{\mu} + \frac{1}{2} + \frac{q^2}{12m^2}\right]. \tag{9.197}$$

where we have introduced the mass parameter μ to make the singular term proportional to m^2 as in $D_1^{\rm sg}$ and $D_2^{\rm sg}$ in (9.142) and (9.149). Apart from the overall factor m^2, the singular term contains a logarithmic dependence on m, in contrast to $D_1^{\rm sg}$ and $D_2^{\rm sg}$, which had only the overall factor m^2. It will turn out that in the present subtraction scheme all terms $m^2\log(m/\mu)$ will eventually cancel in the divergent parts of self-energy and vertex functions. Observe that the singular term this has only a linear q^2-dependence. This is necessary for the renormalizability of the theory, since a q^2-term can be compensated by a counterterm of the type $\partial\phi(x)\partial\phi(x)$ in the Lagrangian density no higher power in the momentum q can. In some textbooks, the factor $\bar{S}_D$ is also expanded in powers of ε. Recalling 5, we see that (9.197) may be written as

$$D_3^{\rm sg}(q) = -\frac{1}{(4\pi)^4}\frac{(m^2)^{1-\varepsilon}}{\varepsilon}\left[\frac{6}{\varepsilon} + 9 - 6\gamma + 6\log 4\pi + \frac{q^2}{2m^2} + \mathcal{O}\left(\varepsilon\right)\right]. \tag{9.198}$$

Consider finally the Feynman integral (9.31):

$$\begin{aligned} 5)\quad I_4(q_i) &= \int \bar{d}^D k_1 \bar{d}^D k_2 \frac{1}{\left(k_1^2+m^2\right)\left[(q_1+q_{12}-k_1)^2+m^2\right]} \\ &\qquad \times \frac{1}{\left(k_2^2+m^2\right)\left[(k_1-k_2+q_3)^2+m^2\right]}. \end{aligned}$$

Thus can be written as

$$I_4(q_i) = \int \bar{d}^D k \frac{1}{k^2+m^2}\frac{1}{(q_1+q_2-k)^2+m^2} I\left(k+q_3\right) \tag{9.199}$$

which becomes using (9.159)

$$\begin{aligned} I_4(q_i) \;=\;& \bar{S}_D\frac{1}{2}\Gamma\left(2-\frac{\varepsilon}{2}\right)\Gamma\left(\frac{\varepsilon}{2}\right)\int_0^1 dx \\ & \times\int \bar{d}^Dk\frac{1}{k^2+m^2}\frac{1}{(q_1+q_2-k)^2+m^2}\frac{1}{\left[(q_3+k)^2x(1-x)+m^2\right]^{\varepsilon/2}}. \end{aligned} \tag{9.200}$$

The denominators are combined via (9.183), and we get

$$\begin{aligned} &\bar{S}_D^2\frac{1}{2}\Gamma\left(2-\frac{\varepsilon}{2}\right)\Gamma\left(2+\varepsilon/2\right)\int_0^1 dx\,[x(1-x)]^{-\varepsilon/2}\int_0^1 dy(1-y)^{\varepsilon/2-1}y \\ &\quad\times\frac{1}{2}\frac{\Gamma\left(2-\varepsilon/2\right)\Gamma(\varepsilon)}{\Gamma\left(2+\varepsilon/2\right)}\int_0^1 dz\Big\{yz(1-yz)(q_1+q_2)^2+y(1-y)q_3^2 \\ &\qquad\qquad -2yz(1-y)q_3(q_1+q_2)+m^2\left[y+\frac{1-y}{x(1-x)}\right]\Big\}^{-\varepsilon}. \end{aligned} \tag{9.201}$$

The only pole term comes from the end-point singularity in the integral at $y=1$. For $y=1$, the curly bracket can be expanded as

$$\begin{aligned} \{\dots\ \} = \left[(q_1+q_2)^2\right]^{-\varepsilon}\Big\{&1-\varepsilon\log\left[z(1-z)+\frac{m^2}{(q_1+q_2)^2}\right] \\ &-\varepsilon\log\frac{[\dots]}{z(1-z)\,(q_1+q_2)^2+m^2}+\mathcal{O}\left(\varepsilon^2\right)\Big\}. \end{aligned} \tag{9.202}$$

Using formula (9.138) with (9.139), the pre-factor of (9.201) is seen to have an expansion

$$\frac{1}{4\varepsilon}(1-\varepsilon)+\mathcal{O}\left(\varepsilon\right),$$

so that

$$\begin{aligned} I_4\left(q_i\right) \;=\;& \bar{S}_D^2\frac{1}{4\varepsilon}(1+\varepsilon)\int_0^1 dx\,[x(1-x)]^{-\varepsilon/2}\int_0^1 dy(1-y)^{\frac{\varepsilon}{2}-1}y \\ &\times\left[(q_1+q_2)^2\right]^{-\varepsilon}\int_0^1 dz\Big\{1-\varepsilon\log\left[z(1-z)+\frac{m^2}{(q_1+q_2)^2}\right] \\ &-\varepsilon\log\frac{[\dots]}{z(1-z)\,(q_1+q_2)^2+m^2}\Big\}+\mathcal{O}(\varepsilon). \end{aligned} \tag{9.203}$$

The first two terms in the integral are independent of x and y, and give

$$\frac{\Gamma^2\left(1-\varepsilon/2\right)}{\Gamma(2-\varepsilon)}\frac{\Gamma\left(\varepsilon/2\right)\Gamma(2)}{\Gamma\left(2+\varepsilon/2\right)}\left[1-\varepsilon L^m\left(q_1+q_2\right)\right], \tag{9.204}$$

where $L^m(q)$ is the integral (9.169) which occurred in the evaluation of $I(q)$of Eq. (9.161)]. Thus, up to here the singular part of $I_4(q_i)$ is

$$I_4\left(q_i\right)=\bar{S}_D^2\frac{\mu^{-2\varepsilon}}{2\varepsilon^2}\left[1-\frac{\varepsilon}{2}-\varepsilon L^m\left(q_1+q_2\right)-\varepsilon\log\frac{(q_1+q_2)^2}{\mu^2}\right]+\mathcal{O}\left(\varepsilon^0\right), \tag{9.205}$$

where we have used the mass parameter μ to make the logarithm dimensionless. We now look at the effect of the last logarithm in (9.202). It is accompanied by a factor ε and it vanishes at $y = 1$ such that it fails to lead to an end-point singularity at $y = 1, \quad \varepsilon = 0$. Therefore it contributes to order $\mathcal{O}(\varepsilon^0)$ and can be neglected as far as the singular parts are concerned. Thus Eq. (9.204) remains unchanged.

Let us decompose this into singular and regular terms in accordance with the decomposition (9.38) using the singular term $I^{\rm sg}$ calculated in (9.166) of the Feynman integral (9.159):

$$\begin{aligned} I_4(q_i) &\equiv I_4^{\rm sg} + I_4^{\rm reg}(q_i) \\ &= \Delta I_4^{\rm sg} + I^{\rm reg}(q_1+q_2)\, I^{\rm sg} + I_4^{\rm reg}(q_i) \end{aligned} \tag{9.206}$$

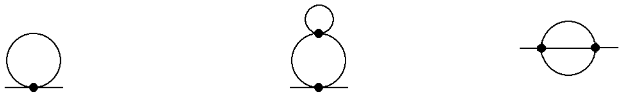
with the momentum-independent term

$$\Delta I_4^{\rm sg} = S_D^2 \frac{\mu^{-2\varepsilon}}{2\varepsilon^2}\left(1 + \frac{\varepsilon}{2}\right). \tag{9.207}$$

9.6 Renormalization of Amplitudes

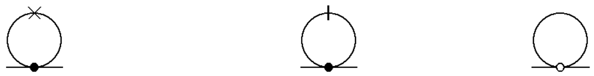
Let us now apply these formulas. Consider at first the self-energy up to second order where we have found it useful to recall grahically the origin of the different contributions.

$$\Sigma(q) = \tfrac{1}{2} g D_1 \qquad - \tfrac{1}{4} g^2 D_2 D_1 \qquad - \qquad \tfrac{1}{6} g^2 D_3$$



$$+ \left(c_1^{m^2} g + c_2^{m^2} g^2 \right) m^2 \quad + \quad \left(c_1^{\phi} g + c_2^{\phi} g^2 \right) q^2$$

$$-\tfrac{1}{2}\, c_1^{m^2} g^2 D_2 \quad -\tfrac{1}{2}\, c_1^{\phi} g^2 \left(D_1 - m^2 D_2 \right) \quad + \tfrac{1}{2}\, c_1^{g} g^2 D_1 \tag{9.208}$$



Obviously, we can regularize this expression in the same way as before by just choosing the singular parts of D_1, D_2, D_2D_1, and D_3 for the counterterms

$$c_1^{m^2} = -\frac{1}{2} D_1^{\rm sg}, \quad c_2^{m^2} = \frac{1}{4}\left(D_2 D_1\right)^{\rm sg} - \frac{1}{4}\left(D_1^{\rm sg} D_2\right)^{\rm sg} - \frac{3}{4}\left(D_2^{\rm sg} D_1\right)^{\rm sg} + \frac{1}{6} D_3^{\rm sg}(0), \tag{9.209}$$

$$c_1^{\phi} = 0, \qquad c_2^{\phi} = \frac{1}{6} D_3'^{\,\rm sg}. \tag{9.210}$$

Care has to be taken to distinguish between the singular parts of $D_2^{\rm sg}D_1$, $D_1^{\rm sg}D_2$, and $(D_2D_1)^{\rm sg}$, and we find from (9.142), (9.144), (9.149), (9.150), and (9.197)

$$\begin{aligned}
(D_1^{\rm sg}D_2)^{\rm sg} &= \bar{S}_D^2\left\{-m^2\mu^{-\varepsilon}\frac{1}{\varepsilon}\cdot(m^2)^{-\varepsilon/2}\left[\frac{1}{\varepsilon}-\frac{1}{2}+\mathcal{O}(\varepsilon)\right]\right\}^{\rm sg},\\
&= \bar{S}_D^2 m^2\mu^{-2\varepsilon}\left[-\frac{1}{\varepsilon^2}+\frac{1}{\varepsilon}\log\frac{m}{\mu}+\frac{1}{2\varepsilon}\right],\\
(D_2^{\rm sg}D_1)^{\rm sg} &= \bar{S}_D^2\left\{\frac{\mu^{-\varepsilon}}{\varepsilon}\cdot(m^2)^{1-\varepsilon/2}\left[-\frac{1}{\varepsilon}+\mathcal{O}(\varepsilon)\right]\right\}^{\rm sg}\\
&= \bar{S}_D^2 m^2\mu^{-2\varepsilon}\left[-\frac{1}{\varepsilon^2}+\frac{1}{\varepsilon}\log\frac{m}{\mu}\right],\\
(D_2D_1)^{\rm sg} &= \bar{S}_D^2\left\{(m^2)^{-\varepsilon/2}\left[\frac{1}{\varepsilon}-\frac{1}{2}+\mathcal{O}(\varepsilon)\right](m^2)^{1-\varepsilon/2}\left[-\frac{1}{\varepsilon}+\mathcal{O}(\varepsilon)\right]\right\}^{\rm sg}\\
&= \bar{S}_D^2 m^2\mu^{-2\varepsilon}\left[-\frac{1}{\varepsilon^2}+\frac{2}{\varepsilon}\log\frac{m}{\mu}+\frac{1}{2\varepsilon}\right],\\
D_3^{\rm sg}(0) &= \bar{S}_D^2 m^2\mu^{-2\varepsilon}\frac{6}{4\varepsilon}\left[-\frac{1}{\varepsilon^2}+\frac{2}{\varepsilon}\log\frac{m}{\mu}-\frac{1}{2\varepsilon}\right], \qquad (9.211)
\end{aligned}$$

In writing (9.210) we have used $I^{\rm sg}=D_2^{\rm sg}$ according (9.174). Due to the non-integer dimension all Feynman integrals carry a factor $\mu^{-\varepsilon}$ for each order in g. It is convenient to absorb these factors, together with the surface factor $\bar{S}_D$, into the coupling constant and introduce the dimensionless *reduced coupling constant*

$$\lambda \equiv g\bar{S}_D\mu^{-\varepsilon}. \qquad (9.212)$$

This considerably simplifies all expressions.[5]

Collecting the different terms in (9.209) and (9.210), we obtain

$$\begin{aligned}
c^{m^2} &= \lambda\frac{1}{2\varepsilon}+\lambda^2\frac{1}{4}\left(\frac{2}{\varepsilon^2}-\frac{1}{2\varepsilon}\right)\\
c^{\phi} &= -\lambda^2\frac{1}{48\varepsilon}. \qquad (9.213)
\end{aligned}$$

Note the pleasant cancellation of all mass factors! This happens at all higher-orders in the coupling constant.

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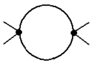
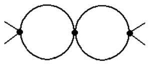
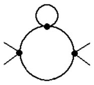
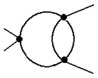
[5] Some people do not include the factor $\bar{S}_D$ into the definition of λ, but only a factor $\bar{S}_4=2/(4\pi)^2$. The relation between the two is obtained form the expansion $\Gamma(D/2)=\Gamma(2-\varepsilon/2)=1+(\gamma-1)\varepsilon/2+\mathcal{O}(\varepsilon^2)$, implying $\bar{S}_D=(2/(4\pi)^2)[1+(\log 4\pi-\gamma+1)\varepsilon/2+\mathcal{O}(\varepsilon^2)]$.

Consider now the coupling constant conterterms. Recalling the full vertex function

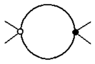
$$\Gamma^{(4)}(q_i) = g \; - \tfrac{1}{2} g^2 \left[I\left(q_1+q_2\right) + 2\,\mathrm{perm} \right] \quad + \tfrac{1}{4} g^3 \left[I^2\left(q_1+q_2\right) + 2\,\mathrm{perm} \right]$$

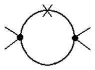
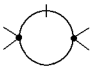
$$+\, \tfrac{1}{2} g^3 \left[I_3\left(q_1+q_2\right) D_1 + 2\,\mathrm{perm} \right] \qquad + \tfrac{1}{2} g^3 \left[I_4(q_i) + 5\,\mathrm{perm} \right]$$

$$+ (c_1^g g + \; c_2^g g^2) g \qquad - \; c_1^g g^3 \left[I\left(q_1+q_2\right) + 2\,\mathrm{perm} \right]$$



$$+ \; c_1^{m^2} g^3 \left[I_3\left(q_1+q_2\right) + 2\,\mathrm{perm} \right] \qquad + \; c_1^{\phi} g^3 \left[I_3\left(q_1+q_2\right) + 2\,\mathrm{perm} \right]$$

$$(9.214)$$

we may identify

$$c_1^g \;=\; \frac{3}{2} I^{\mathrm{sg}} \tag{9.215}$$

$$\begin{aligned} c_2^g \;=\; & -\frac{1}{4}\left[\left(I^2\right)^{\mathrm{sg}} + 2\ \mathrm{perm} \right] - \frac{1}{2}\left[(I_3 D_1)^{\mathrm{sg}} + 2\ \mathrm{perm} \right] - \frac{1}{2}\left[I_4^{\mathrm{sg}} + 5\ \mathrm{perm} \right] \\ & + \frac{3}{2}\left[(I^{\mathrm{sg}} I)^{\mathrm{sg}} + 2\ \mathrm{perm} \right] + \frac{1}{2}\left[(D_1^{\mathrm{sg}} I_3)^{\mathrm{sg}} + 2\ \mathrm{perm} \right]. \end{aligned} \tag{9.216}$$

Inserting (9.206) into (9.216) we separate $I = I^{\mathrm{sg}} + I^{\mathrm{reg}}$, $D_1 = D_1^{\mathrm{sg}} + D_1^{\mathrm{reg}}$ and use the fact that $I_3(q_i)$ is regular to cancel the term $(I_3 D_1)^{\mathrm{sg}}$ against the term $-(D_1^{\mathrm{sg}} I_3)^{\mathrm{sg}}$, so that

$$\begin{aligned} c_2^g \;=\; & -\frac{3}{4}\left[(I^{\mathrm{sg}})^2 + 2 I^{\mathrm{sg}} I^{\mathrm{reg}} \right] - 3\left(\Delta I_4^{\mathrm{sg}} + I^{\mathrm{sg}} I^{\mathrm{reg}} \right) \\ & + \frac{9}{2}\left[(I^{\mathrm{sg}})^2 + I^{\mathrm{sg}} I^{\mathrm{reg}} \right]. \end{aligned} \tag{9.217}$$

The terms containing I^{reg} are seen to cancel each other, and we arrive at

$$c_2^g = \frac{15}{4}\left(I^{\mathrm{sg}}\right)^2 - 3\Delta I_4^{\mathrm{sg}}. \tag{9.218}$$

We now insert (9.174), (9.207), and obtain

$$\begin{aligned} c^g \;&=\; \lambda \frac{3}{2\varepsilon} + \lambda^2 \left[\frac{15}{4}\frac{1}{\varepsilon^2} - 3\left(\frac{1}{2\varepsilon^2} + \frac{1}{4\varepsilon} \right) \right] \\ &=\; \lambda \frac{3}{2\varepsilon} + \lambda^2 \frac{1}{4}\left(\frac{9}{\varepsilon^2} - \frac{3}{\varepsilon} \right). \end{aligned} \tag{9.219}$$

Here we have to pause for a very important observation. Nowhere in the formulas for c^{m^2}, c^{ϕ}, c^{g} does the physical mass appear. There is only the arbitrary mass scale which has been used up to make the coupling constant dimensionless. If this situation prevails to all orders in perturbation theory we can conclude: The counterterms calculated according to the rules of this section can be used to renormalize massive as well as massless theories. The multiplicative renormalization constants depend only on the dimensionless coupling constant g.

The finite regularized vertex functions depend on the choice of g, m and the parameter μ. For massive theories μ can be set equal to m and only the two parameters g, m are necessary to specify the manifold of all perturbative solutions to the ϕ^4 field theory. For zero physical mass, the parameter μ can no longer be eliminated. Now the vertex functions will depend on g and μ. Since the parameter μ was introduced in a completely arbitrary manner, we have the suspicion that it cannot represent a true degree of freedom in the calculation of both massive and massless theories. In fact we shall see in the next section that there is only a two parameter manifold in g, m, μ space which corresponds to different sets of vertex functions. As far as the renormalization is concerned, however, μ is absolutely necessary to obtain finite expressions if the physical mass m is taken to zero.

9.7 Generalization to O(N)-Symmetric Model

In many physical systems, the field ϕ has several degrees of freedom: In the superconductor it is a complex field which may be considered as a two-component object with ϕ^2, ϕ^4 replaced by

$$\begin{aligned} \phi^2 &\rightarrow |\phi|^2 = \phi_1^2 + \phi_2^2 \\ \phi^4 &\rightarrow |\phi|^4 \rightarrow \left(\phi_1^2 + \phi_2^2\right)^2 . \end{aligned} \tag{9.220}$$

A magnetic system, on the other hand, is characterized by a vector field (ϕ_1, ϕ_2, ϕ_3) and the Lagrangian contains the invariants

$$\begin{aligned} \phi^2 &\rightarrow \phi_1^2 + \phi_2^2 + \phi_3^2 \\ \phi^4 &\rightarrow \left(\phi_1^2 + \phi_2^2 + \phi_3^2\right)^2 . \end{aligned} \tag{9.221}$$

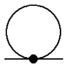
It is therefore useful to generalize all results to the case of an O(N)-vector ϕ_a such that instead of ϕ^2, ϕ^4 we have:

$$\begin{aligned} \phi^2 &\rightarrow \sum_{a=1}^{N} \phi_a^2 \\ \phi^4 &\rightarrow \left(\sum_{a=1}^{N} \phi_a^2\right)^2 . \end{aligned} \tag{9.222}$$

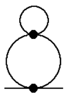
The propagator is the same as before except it is accompanied by a Kronecker δ_{ab}. The vertex function, on the other hand, carries a symmetric tensor

$$T_{abcd} = \frac{1}{3}\left(\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}\right) . \tag{9.223}$$

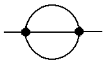
When calculating the Feynman diagrams, all integrations remain the same except that each integral is accompanied by a product of T-tensors with a contraction of indices for every internal line. For the previous diagrams these may be given as follows:



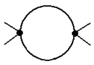
$$D_1 \to D_1 T_{\underline{ab}cc},$$



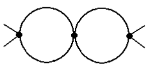
$$D_2 D_1 \to D_2 D_1 T_{\underline{ab}cd} T_{cdee},$$



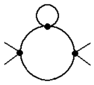
$$D_3 \to D_3 T_{\underline{a}cde} T_{\underline{b}cde},$$



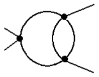
$$I \to I T_{\underline{ab}ef} T_{\underline{cd}ef}, \tag{9.224}$$



$$I^2 \to I^2 T_{\underline{ab}ef} T_{efgh} T_{gh\underline{cd}},$$



$$I_3 D_1 \to I_3 D_1 T_{\underline{ab}ef} T_{\underline{cd}eg} T_{fghh},$$



$$I_4 \to I_4 T_{\underline{ab}ef} T_{e\underline{c}gh} T_{f\underline{d}gh}.$$

For greater transparency we have underlined the external indices.

It is convenient to introduce the reduced matrix elements of the contracted tensors as follows

$$\begin{aligned}
&T_{abcc} = \delta_{ab} T_{D_1},\\
&T_{abcd} T_{cdee} = \delta_{ab} T_{D_2 D_1} = \delta_{ab} T_{D_1}^2,\\
&T_{acde} T_{bcde} = \delta_{ab} T_{D_3},\\
&T_{abef} T_{cdef}\big|_{\rm symm} = T_{abcd} T_I,\\
&T_{abef} T_{efgh} T_{cdgh}\big|_{\rm symm} = T_{abcd} T_{I^2},\\
&T_{abef} T_{cdeg} T_{fghh}\big|_{\rm symm} = T_{abcd} T_{I_3 D_1} \equiv T_{abcd} T_I T_{D_1},\\
&T_{abef} T_{ecgh} T_{fdgh}\big|_{\rm symm} = T_{abcd} T_{I_4}.
\end{aligned} \tag{9.225}$$

The symbol symm denotes symmetrization in the indices abcd which replaces each $\delta_{ab}\delta_{cd}$ by T_{abcd}. In order to calculate the irreducible matrix elements we observe that

$$T_{abcc} = \frac{N+2}{3}\delta_{ab}, \tag{9.226}$$

$$T_{aefg}T_{befg} \;=\; \frac{N+2}{3}\delta_{ab}, \tag{9.227}$$

so that

$$T_{D_1} \;=\; \frac{N+2}{3}, \tag{9.228}$$

$$T_{D_3} \;=\; \frac{N+2}{3}. \tag{9.229}$$

In order to calculate T_I we first note that

$$T_{abef}T_{cdef} = \frac{1}{9}\left[(N+4)\,\delta_{ab}\delta_{cd} + 2\delta_{ac}\delta_{bd} + 2\delta_{ad}\delta_{bc}\right]. \tag{9.230}$$

It is useful to abbreviate the three tensors in the brackets as $A_1,\ A_2,\ A_3$, i.e., we write

$$T_{abef}T_{cdef} = \left[\frac{N+4}{9}A_1 + \frac{2}{9}A_2 + \frac{2}{9}A_3\right]_{abcd}. \tag{9.231}$$

The symmetrization of the tensors $A_1,\ A_2,\ A_3$ gives each time T_{abcd} so that

$$T_{abcf}T_{cdef}|_{\rm symm} = \frac{N+8}{9}T_{abcd} \tag{9.232}$$

and hence

$$T_I = \frac{N+8}{9}. \tag{9.233}$$

For the other products (9.225) we observe the multiplication rules

$$\begin{aligned}&(p_1A_1 + p_2A_2 + p_3A_3)_{abef}\,(q_1A_1 + q_2A_2 + q_3A_3)_{\rm efcd} \\ &\quad = \left\{\left[p_1\left(q_1N + q_2 + q_3\right) + p_2q_1 + p_3q_1\right]A_1 + \left(p_2q_2 + p_3q_3\right)A_2 + \left(p_2q_3 + p_3q_2\right)A_3\right\}_{abcd}.\end{aligned} \tag{9.234}$$

If we want to form $T_{abef}T_{efgh}T_{cdgh}$, we have to multiply $A_1 + A_2 + A_3$ by $\frac{N+4}{9}A_1 + \frac{2}{9}A_2 + \frac{2}{9}A_3$ and symmetrize the result which gives

$$\frac{1}{3}\left(\frac{N+4}{9}N + \frac{4}{9}\right) + \frac{2}{3}\left(\frac{N+4}{9} + \frac{2}{9} + \frac{2}{9}\right)T_{abcd} \tag{9.235}$$

and hence

$$T_{I^2} = \frac{1}{27}\left(N^2 + 6N + 20\right). \tag{9.236}$$

The last product in (9.225) is found by using the general rule

$$\begin{aligned}&(p_1A_1 + p_2A_2 + p_3A_3)_{abcd}\,(q_1A_1 + q_2A_2 + q_3A_3)_{cedf} \\ &\qquad = \left\{\left[p_1\left(q_1 + Nq_2 + q_3\right) + \left(p_2 + p_3\right)q_2\right]A_1 \right. \\ &\qquad\qquad \left.\left(p_2q_1 + p_3q_3\right)A_2 + \left(p_3q_1 + p_2q_3\right)A_3\right\}_{abef}.\end{aligned} \tag{9.237}$$

Applying this to $\frac{1}{3}(A_1+A_2+A_3)$ and $\frac{N+4}{9}A_1+\frac{2}{9}A_2+\frac{2}{9}A_3$ we find, after symmetrization

$$\begin{aligned} T_{I_4} &= \frac{1}{3}\left(\frac{N+4}{9}+N\frac{2}{9}+\frac{2}{9}\right)+\frac{1}{3}\left(\frac{2}{9}+\frac{2}{9}\right)+2\frac{1}{3}\left(\frac{N+4}{9}+\frac{2}{9}\right) \\ &= \frac{1}{27}(5N+22)\,. \end{aligned} \tag{9.238}$$

Diagrams D_2D_1 and I_3D_1 in Eq. (9.224) have only a single loop attached to a line. Any such attachment inserts a tensor (9.226) into one of the index contractions, producing merely a factor $(N+2)/3$. Thus we obtain

$$T_{D_2D_1} = \left(\frac{N+2}{3}\right)^2 \tag{9.239}$$

$$T_{I_3D_1} = \left(\frac{N+8}{9}\right)\left(\frac{N+2}{3}\right). \tag{9.240}$$

Let us now consider the counterterms (9.209) and (9.210) in the presence of T-tensors. They become

$$\begin{aligned} (c_1^{m^2})_{\alpha\beta} = -\frac{1}{2}D_1^{\text{sg}}T_{D_1}\delta_{\alpha\beta},\quad (c_2^{m^2})_{\alpha\beta} &= \frac{1}{4}(D_2D_1)^{\text{sg}}\,T_{D_2D_1}\delta_{\alpha\beta}-\frac{1}{4}(D_1^{\text{sg}}D_2)^{\text{sg}}\,T_{D_1}T_{\alpha\beta\gamma\gamma} \\ &\quad -\frac{3}{4}(D_2^{\text{sg}}D_1)^{\text{sg}}\,T_IT_{\alpha\beta\gamma\gamma}+\frac{1}{6}D_3^{\text{sg}}(0)\,T_{D_3}\delta_{\alpha\beta}, \end{aligned} \tag{9.241}$$

$$(c_1^{\phi})_{\alpha\beta} \;=\; 0, \qquad\qquad (c_2^{\phi})_{\alpha\beta} \;=\; \frac{1}{6}D_3'^{\,\text{sg}}\,T_{D_3}\delta_{\alpha\beta}. \tag{9.242}$$

Inserting into (9.242) the relations $T_{D_1}T_{\alpha\beta\gamma\gamma}=T_{D_1}^2\delta_{\alpha\beta}$, $T_IT_{\alpha\beta\gamma\gamma}=T_{D_2}T_{D_1}\delta_{\alpha\beta}$, and going over to the dimensionless coupling constant $\lambda = gS_D\mu^{-\varepsilon}$ of Eq. (9.212), we obtain the generalization of Eqs. (9.213):

$$\begin{aligned} c^{m^2} &= \lambda\frac{1}{2\varepsilon}T_{D_1}+\frac{\lambda^2}{4}\left[\frac{1}{\varepsilon^2}T_{D_2D_1}+\left(\frac{1}{\varepsilon^2}-\frac{1}{2\varepsilon}\right)T_{D_3}\right], \\ c^{\phi} &= -\lambda^2\frac{1}{48\varepsilon}T_{D_3}, \\ c^{g} &= \frac{3}{2\varepsilon}\lambda T_I+\lambda^2\left[\frac{3}{4}\frac{1}{\varepsilon^2}T_{I^2}+3\left(\frac{1}{2\varepsilon^2}+\frac{1}{4\varepsilon}\right)T_{I_4}\right]. \end{aligned} \tag{9.243}$$

For the counterterms (9.215) and (9.218) we find similarly

$$(c_1^{g})_{\alpha\beta\gamma\delta} \;=\; \frac{3}{2}I^{\text{sg}}T_IT_{\alpha\beta\gamma\delta} \tag{9.244}$$

$$\begin{aligned} (c_2^{g})_{\alpha\beta\gamma\delta} \;=\; &\left\{-\frac{3}{4}\left(I^2\right)^{\text{sg}}T_{I^2}-\frac{3}{2}(I_3D_1)^{\text{sg}}\,T_IT_{D_1}-3(I_4)^{\text{sg}}T_{I_4}\right. \\ &\left.+\frac{9}{2}(I^{\text{sg}}I)^{\text{sg}}\,T_{I^{\text{sg}}I}+\frac{3}{2}(D_1^{\text{sg}}I_3)^{\text{sg}}\,T_{D_1^{\text{sg}}I_3}\right\}T_{\alpha\beta\gamma\delta}, \end{aligned} \tag{9.245}$$

where

$$T_{I^{\text{sg}}I}T_{\alpha\beta\gamma\delta}=T_IT_{\alpha\beta\sigma\tau}T_{\sigma\tau\gamma\delta}=T_I^2T_{\alpha\beta\gamma\delta},\qquad T_{D_1^{\text{sg}}I_3}=T_{D_1}T_{\alpha\beta\sigma\tau}T_{\sigma\tau\gamma\delta}=T_{D_1}T_IT_{\alpha\beta\sigma\tau}. \tag{9.246}$$

The resulting generalization of (9.215) is

$$\begin{aligned} c_2^g &= -\frac{3}{4}\left[(I^{\rm sg})^2+2I^{\rm sg}I^{\rm reg}\right]T_{I^2}-3\left(\Delta I_4^{\rm sg}+I^{\rm sg}I^{\rm reg}\right)T_{I_4}\\ &\quad+\frac{9}{2}\left[(I^{\rm sg})^2+I^{\rm sg}I^{\rm reg}\right]T_I^2. \end{aligned} \tag{9.247}$$

With the reduced matrrix elements (9.233) and (9.238), the regular terms $I^{\rm reg}$ cancel as before (here somewhat more miraculously), and c_2^g simplifies to

$$c_2^g=(I^{\rm sg})^2\left(\frac{9}{2}T_{I_4}-\frac{3}{4}T_I^2\right)-3\Delta I_4^{\rm sg}\,T_{I_4}. \tag{9.248}$$

Inserting the reduced matrix elements (9.232)–(9.238), and the reduced coupling constant $\lambda=\tilde g S_D\mu^{-\varepsilon}$ of Eq. (9.212), the counterterms become, finally,

$$\begin{aligned} c^{m^2} &= \lambda\frac{1}{2\varepsilon}\frac{N+2}{3}+\lambda^2\left[\frac{1}{4\varepsilon^2}\left(\frac{N+2}{3}\right)^2-\frac{1}{4}\left(\frac{1}{\varepsilon^2}-\frac{1}{2\varepsilon}\right)\frac{N+2}{3}\right],\\ c^{\phi} &= -\lambda^2\frac{1}{48\varepsilon}\frac{N+2}{3},\\ c^{g} &= \lambda\frac{3}{2\varepsilon}\frac{N+8}{9}+\lambda^2\left\{\frac{3}{4}\frac{1}{\varepsilon^2}\frac{N^2+6N+20}{27}+3\left(\frac{1}{2\varepsilon^2}+\frac{1}{4\varepsilon}\right)\frac{5N+22}{27}\right\}. \end{aligned} \tag{9.249}$$

A further generalization which is sometimes encountered in the literature and which is useful for applications is the case of n fields ϕ_i^α $(i=1,\dots,n)$ each of which occur in an O(q)-symmetric combination

$$\mathcal{L}=\frac{1}{2}\sum_{i,\alpha}^{n,q}\left[(\partial\phi_i^\alpha)^2+m^2(\phi_i^\alpha)^2\right]+\frac{1}{4!}\sum_{i,j,k,l=1}^{n}g_{ijkl}\sum_{\alpha=1}^{q}\phi_i^\alpha\phi_j^\alpha\sum_{\beta=1}^{q}\phi_k^\beta\phi_l^\beta. \tag{9.250}$$

Among these, the case of a cubic symmetry in the indices is of special interest when there are only two independent couplings

$$\sum_{i,i'=1}^{n}g_{ii'}\sum_{\alpha=1}^{q}(\phi_i^\alpha)^2\sum_{\beta=1}^{q}(\phi_i^\beta)^2=g_1\left(\sum_{i=1}^{n}\sum_{\alpha=1}^{q}(\phi_i^\alpha)^2\right)^2+g_2\sum_{i=1}^{n}\left(\sum_{\alpha=1}^{q}(\phi_i^\alpha)^2\right)^2. \tag{9.251}$$

The special case of n complex fields (i. e. ϕ_i^α with $\alpha=1,2$ governs the statistical mechanics of ensembles of dislocation lines in a crystal. They also are used to describe phase transforms in cubic crystals. The interaction (9.257) corresponds to the tensor (9.223) being replaced by

$$\begin{aligned} T_{i\alpha,i\beta,k\gamma,l\delta} &= g_1S_{i\alpha,j\beta,k\gamma,l\delta}+g_2F_{i\alpha,j\beta,k\gamma,l\delta}\\ &= \frac{g_1}{3}\left(\delta_{ij}\delta_{kl}\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{ik}\delta_{jl}\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{il}\delta_{jk}\delta_{\alpha\delta}\delta_{\beta\gamma}\right)\\ &+\ \frac{g_2}{3}\left(\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}\right)\delta_{ij}\delta_{ik}\delta_{il}. \end{aligned} \tag{9.252}$$

It is then straightforward to generalize the previous results. Take, for example, T_I arising from

$$T_{abef}T_{cdef}|_{\text{symm}} = T_{abcd}T_I. \tag{9.253}$$

Multiplying the tensors S, F with each other we find

$$\begin{aligned} SS|_{\text{symm}} &= \frac{nq+8}{9}S, \\ FF|_{\text{symm}} &= \frac{q+8}{9}F, \\ FS|_{\text{symm}} &= \frac{2}{3}F + \frac{q+2}{9}S. \end{aligned} \tag{9.254}$$

Hence, the lowest-order counterterms $c^g = \frac{2}{3}\lambda T_I$ are replaced by

$$\begin{aligned} c^{g_1} &= \frac{3}{2\varepsilon}\left(\frac{pq+8}{9}\lambda_1 + 2\frac{q+2}{9}\lambda_2\right), \\ c^{g_2} &= \frac{3}{2\varepsilon}\left(\frac{q+8}{9}\lambda_1 + \frac{4}{3}\lambda_2\right). \end{aligned} \tag{9.255}$$

9.8 Finite S-Matrix Elements

We are now in a position to calculate also finite S matrix elements. Again for simplicity we shall consider here only elastic scattering between two ϕ-particles, the generalization being straight-forward.

Recalling Eq. (8.74), the four-point function $G^{(4)}(x_1, \ldots, x_n)$ has the following structure: It consists of disconnected and connected parts with the disconnected ones being the product of two interacting single-particle Green functions: We may write

$$G^{(4)}(x_4,x_3,x_2,x_1) = \left[G^{(2)}(x_4,x_3)G^{(2)}(x_2,x_1) + 2\text{ perm}\right] + G_c^{(4)}(x_4,x_3,x_2,x_1). \tag{9.256}$$

The two-particle Green functions were obtained by summing the one-particle irreducible graphs of the self energy (see (9.26)) and forming the geometric series in momentum space

$$G^{(2)}(q) = \frac{i}{q^2 - m^2 - \Sigma(q) + i\eta}. \tag{9.257}$$

The connected four-point function is then obtained

$$G^{(4)}(q_4,q_3,q_2,q_1) = G^{(2)}(q_n)G^{(2)}(q_3)\Gamma^{(4)}(q_4,q_3,q_2,q_1)G^{(2)}(q_2)G^{(2)}(q_1), \tag{9.258}$$

where $\Gamma^{(4)}$ is the sum of all one-particle irreducible vertex graphs. We shall now prove that $\Gamma^{(4)}$ gives directly the scattering amplitude if the momenta q_4, q_3, q_2, q_1, are taken to the physical mass shell values of incoming and outgoing particles.[6] The argument proceeds very similar to the previous discussion in Section (8.7). We form again the limit (8.99) but with the energies q_i^0 on the physical mass shells (rather than the bare mass shells used there). We are then confronted with studying the limit (8.100) not with the free but the fully interaction two-point function $G^{(2)}(q)$

$$\lim_{x_1^0\to-\infty}\sqrt{\frac{2q_1^0}{V}}e^{-i(q_1^0x_1^0-\mathbf{q}_1\mathbf{x}_1)}\int\frac{d^4q}{(2\pi)^4}e^{-iq(z-x)}\frac{i}{q^2-m^2-\Sigma(q)+i\eta}. \qquad (9.259)$$

The integrand has poles at the physical energy value $q^0=\pm\sqrt{\mathbf{q}^2+m^2}\mp i\eta$. In addition there are cuts from the higher Feynman amplitudes, the lowest starting at $q_0=\sqrt{\mathbf{q}^2+(3m)^2}$ from the second-order graph . The cuts are slightly displaced in the imaginary direction due to the $i\eta$ attached with each mass. Thus the complex q_0 plane looks as shown in Fig. 9.1. If we now distort the contour of q^0 integration we pick up contribution of the pole at $q^0=\sqrt{\mathbf{q}^2+m^2}$ as well as the cut. But in the limit $x_1^0\to-\infty$ only the pole contributes since at the cut q^0 and q_1^0 do not cancel and an infinitely rapid oscillation remains which is equivalent to zero by the standard argument. Thus we obtain the same rules as before but now for $G^{(2)}$ rather than $G_0^{(2)}$ and with the particles on the physical mass shell. As a consequence, the four-point function (9.258) gives the following S-matrix element

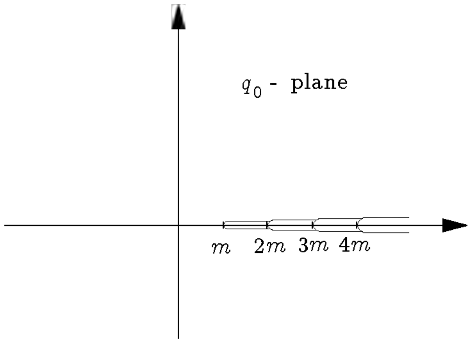


FIGURE 9.1 Singularities in complex q_0-plane of Feynman propagator. There are poles and cuts due to three- and more-particle intermediate states in the diagram.

$$\begin{aligned} S\left(q_4q_3|q_2q_1\right) &= \delta_{q_3q_1}\delta_{q_4q_2}+\delta_{q_3q_2}\delta_{q_4q_1} \\ &+ (2\pi)^4\delta^{(4)}\left(q_4+q_3-q_2-q_1\right)\prod_{i=1}^{4}\frac{1}{\sqrt{2Vq_i^0}}\Gamma^{(4)}\left(q_1,q_3,q_2,q_1\right), \end{aligned} \qquad (9.260)$$

with $\Gamma^{(4)}$ being the amputated OPI four-point function. The first two terms correspond to the particles running past each other without scattering (the so-called *direct beam* right behind the sample in the experiment). The symmetrization in q_3q_4

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[6] Remember that $\Gamma\left(q_4,q_3,q_2,q_1\right)$ are defined for any off-shell value of the energy $q_i^0\neq\sqrt{\mathbf{q}_i^2+m^2}$.

is a reflection of particle identity. The second term contains the amplitude for true scattering. The factor after the total momentum conservation $(2\pi)^4\delta^{(4)}\left(p_f - p_i\right)$ function is often referred to as T-matrix.

In a scattering process where two particles enter and four emerge (a so called production process), the disconnected part is absent and we have directly

$$S\left(q_6 q_5 q_4 q_3 | q_2 q_1\right) = (2\pi)^4\delta^{(4)}\left(\sum_{i=3}^{6} q_i - \sum_{i=1}^{2} q_i\right) i\Gamma^{(6)}\left(q_6, q_5, q_4, q_3, q_2, q_1\right)\prod_{i=1}^{6}\frac{1}{\sqrt{2Vq_i^0}} \tag{9.261}$$

Appendix 9A Alternative Proof of Veltman's Integral Rule

Here we shall convince ourselves in another way of the consistency of Veltman's integral rule (9.127):

$$\int d^D k k^{-2\nu} = 0, \qquad D < 2\nu, \tag{9A.1}$$

In Eq. (9.219), this was derived by taking the limit $m \longrightarrow 0$ in the dimensionally regularized integral (9.122) for $D > 2\nu$. Instead of the integral (9A.1), we shall discuss the more general integral

$$\int d^D k\, f(k), \tag{9A.2}$$

with a rotationally invariant $f(k)$ which is bounded for large k by

$$|f(k)| < A\, k^{-2\nu}. \tag{9A.3}$$

Then the integral exists for $0 < D < 2\nu$ whereas it is not immediately defined for $-2 < D < 0$ since, after integrating out the angular variables, the integrand has an IR-singularity at $k = 0$:

$$\int d^D k\, f(k) \;\equiv\; S_D \int_0^\infty dk\, k^{D-1} f(k)\ .$$

This singularity can be circumvented by the same trick as the singularity at $\tau = 0$ in the integral (9.120). With some $c > 0$ we rewrite

$$\begin{aligned}\int d^D k f(k) \;&=\; S_D\left\{\int_c^\infty dk\, k^{D-1} f(k)\right.\\ &\qquad \left. + \int_0^c dk\, k^{D-1}[f(k) - f(0)]\right\} + f(0)\frac{c^D}{D}.\end{aligned} \tag{9A.4}$$

This is independent of c and defined for $-2 < D < 2\alpha$. In the limit $c \longrightarrow 0$ it gives back the previous integral defined only for $0 < D < 2\alpha$. For $-2 < D < 0$ we can take the opposite limit $c \longrightarrow \infty$ and only the second term survives.

$$\int d^D k f(k) = \int d^D k[f(k) - f(0)]. \tag{9A.5}$$

For $D \to 0$, the third term gives

$$\int d^0 k f(k) = f(0). \tag{9A.6}$$

Repeated application of this procedure permits a continuation of the integral to arbitrarily low dimensions $-2l-2 < D < -2l$ ($l = 0, 1, 2, \ldots$) via the formula

$$\int d^D k f(k) = \int d^D k \left\{[f(k) - f(0)] - k^2 f'(0) - \ldots - k^{2l} f^{(l)}(0)\right\}. \tag{9A.7}$$

with

$$\int d^{-2l} k f(k) = (-\pi)^{-l} f^{(l)}(0). \tag{9A.8}$$

Note that if an integral has initially no range of D where it exists, such as with the function $f(k) = k^{-2\nu}(k^2+a)/(k^2+b)$, the above procedure serves to define it for $-2l + 2\nu < D < 2\nu$ ($l = 1, 2, 3, \ldots$). With $l = 1$, for example, we define

$$\begin{aligned} \int d^D k k^{-2\nu} \frac{k^2+a}{k^2+b} &\equiv \int d^D k k^{-2\nu} \left(\frac{k^2+a}{k^2+b} - \frac{a}{b}\right) \\ &= \int d^D k k^{-2\nu} \frac{b-a}{b} \frac{k^2}{k^2+b}, \end{aligned} \tag{9A.9}$$

with the right-hand side existing for $-2 + 2\nu < D < 2\nu$.

We now observe that this continuation procedure can make sense only if the difference between the two sides is formally equal to zero, i.e., if

$$\int d^D k k^{2\nu} = 0, \quad D < 2\nu. \tag{9A.10}$$

The basic reason for this identity is, of course, the fundamental requirement of dimensional regularization that the Gaussian integral (9.118) was assumed to hold for all D, positive and negative values. Setting q and m equal to zero this implies

$$\int d^D k e^{-\tau k^2} = \left(\frac{\pi}{\tau}\right)^{D/2}. \tag{9A.11}$$

For $D < 0$ the limit $\tau \to 0$ gives once more (9.123) while for $D = 0$ we obtain (9A.6). Inserting a factor $k^{-2\nu}$ we have

$$\int d^D k k^{-2\nu} e^{-\tau k^2} = \frac{\Gamma(D/2 - \nu)}{\Gamma(D/2)} \pi^{D/2} \tau^{\nu - D/2}. \tag{9A.12}$$

For $D < 2\nu$ the limit $\tau \to 0$ gives

$$\int d^D k k^{-2\nu} = 0, \tag{9A.13}$$

in agreement with (9A.10).

Note that this relation implies a specific choice af a small-k cutoff. Suppose we had regularized the small-k regime of the Gaussian integral by an exponential cutoff $e^{-\delta/k^2}$. Then we would have obtained

$$\int d^D k k^{-2\nu} e^{-\tau k^2-\delta/k^2} = \frac{\Gamma(D/2-\nu)}{\Gamma(D/2)} \frac{\pi^{D/2}}{\tau^{D/2-\nu}} 2\sqrt{\tau\delta} K_{D/2-\nu}(2\sqrt{\tau\delta}). \tag{9A.14}$$

where $K_\nu(z)$ is the modified Bessel function. For small z this behaves like

$$K_\nu(z) = K_{-\nu}(z) \approx \frac{1}{2}\Gamma(\nu)\left(\frac{z}{2}\right)^\nu, \tag{9A.15}$$

so that for small τ and δ the integral would have been

$$\int d^D k k^{-2\nu} e^{-\tau k^2-\delta/k^2} \approx \frac{\Gamma(D/2-\nu)}{\Gamma(D/2)} \pi^{D/2} \begin{cases} \dfrac{\pi^{D/2}}{\tau^{D/2-\nu}}, & D > 2\nu, \\ \dfrac{\pi^{D/2}}{\delta^{D/2-\nu}}, & D < 2\nu, \end{cases} \tag{9A.16}$$

with the limit $\tau \to 0$ no longer giving zero for $D < 2\nu$ but a very large number. In a renormalizable massless theory this infinity must cancel order by order in parturbation theory. It is this prpperty which makes it possible to use the infrared cutoff implied by the integral formula $\int d^D k k^{-2\nu} = 0$ also for $D > 2\nu$.

Notes and References

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10

Quantum Electrodynamics

In Chapter 4 we have learned how to quantize relativistic free fields and in Chapters 5, 6 how to deal with interactions perturbatively if the coupling is small. Fortunately, there is a large set of physical phenomena for which the techniques developed so far are powerful enough to supply theoretical results to be compared with observable quantities. These, moreover, turn out to be in extremely good agreement with the experimental measurements. It is the quantized theory of interacting electrons and photons called *quantum electrodynamics* or shortly QED.

10.1 Gauge Invariant Interacting Theory

The free Lagrangians of electrons and the photons are known from Chapter 5 as

$$\mathcal{L}(x) = \overset{\text{el}}{\mathcal{L}}(x) + \overset{\text{ph}}{\mathcal{L}}(x) \tag{10.1}$$

with

$$\begin{aligned} \overset{\text{el}}{\mathcal{L}}(x) &= \bar{\psi}(x)\,(i\partial\!\!\!/ - m)\,\psi(x) && (10.2)\\ \overset{\text{ph}}{\mathcal{L}}(x) &= -\frac{1}{4}F_{\mu\nu}^2(x) = -\frac{1}{4}\left[\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)\right]^2 && (10.3) \end{aligned}$$

When quantizing the photon theory, there were subtleties due to the gauge freedom in the choice of the gauge fields A_μ:

$$A_\mu(x) \to A_\mu(x) + \partial_\mu\Lambda(x). \tag{10.4}$$

For this reason, there are different ways of constructing a Hilbert space of free particles:

The first [see Subsec. 5.1.2 was based on a quantization of only the two physical transverse degrees of freedom. The time component of the gauge field A^0 and the spatial divergence $\boldsymbol{\nabla}\cdot\mathbf{A}(x)$ had no canonically conjugate field and were therefore classical fields which had no manifestation at all in the Hilbert space. The two were related by Coulomb's law which in the absence of charges reads

$$\boldsymbol{\nabla}^2 A^0(x) = -\partial^0\boldsymbol{\nabla}\cdot\mathbf{A}(x). \tag{10.5}$$

Only the *transverse* components, defined by

$$A^i_\perp(x) \equiv \left(\delta^{ij} - \nabla^i\nabla^j/\boldsymbol{\nabla}^2\right) A^j(\mathbf{x}, t) \tag{10.6}$$

became operators. These components represent the proper dynamical variables of the system. After quantization, the positive and negative frequency parts of these fields defined creation and annihilation operators for the electromagnetic quanta, the photons of right and left circular polarization.

This method had an esthetical disadvantage that two of the four components of the vector field $A^\mu(x)$ required a different treatment. The components which become operators change with the frame of reference in which the canonical quantization procedure is performed.

To circumvent this, a second quantization procedure was presented which, at first sight, looked somewhat contrived. It started out by modifying the initial photon Lagrangian by a gauge-fixing term

$$\mathcal{L}_{\rm GF}(x) = -D\partial^\mu A_\mu(x) + \alpha D^2(x)/2. \tag{10.7}$$

In the Gupta-Bleuler quantization scheme, the propagator took a pleasant covariant form. But this was at the expense of another disadvantage was that this Lagrangian describes the propagation of four particles of which only two correspond to physical states. Accordingly, the Hilbert space contained two kinds of unphysical particle states, states with negative and with zero norm. Still, a physical interpretation of the formalism was found by means of a subsidiary condition selecting the physical subspace in the Hilbert space of free particles.

10.1.1 Reminder of Classical Electrodynamics of Point Particles

In this chapter we want to couple electrons and photons with each other by an appropriate interaction term and study the resulting interacting field theory which is the famous quantum electrodynamics. Since the coupling should not change the two physical degrees of freedom described by the four-component photon field A^μ it is important to preserve the gauge invariance which was so essential in assuring the correct Hilbert space. The prescription how this can be done has been known for a long time in the classical electrodynamics of point particles: There, a free relativistic particle moving along an arbitrary parametrized path $x^\mu(\tau)$ in four-space is described by an action

$$\mathcal{A} = -mc^2 \int d\tau \sqrt{\frac{dx^\mu}{d\tau}\frac{dx_\mu}{d\tau}} = -mc^2 \int dt \left[1 - \frac{\mathbf{v}^2(t)}{c^2}\right]^{1/2}, . \tag{10.8}$$

where $x^0(\tau) = t$ is the time and $d\mathbf{x}/dt = \mathbf{v}(t)$ the velocity along the path. If the particle has a charge e and lies at rest at position $\mathbf{x}$, its potential energy is

$$V(t) = e\phi(\mathbf{x}, t) \tag{10.9}$$

where

$$\phi(\mathbf{x},t)=A^0(\mathbf{x},t). \tag{10.10}$$

In our convention, the charge of the electron e has a negative value to have agreement with the sign in the historic form of the Maxwell equations

$$\begin{aligned}\boldsymbol{\nabla}\cdot\mathbf{E}(x) &= -\boldsymbol{\nabla}^2\phi(x)=\rho(x),\\ \boldsymbol{\nabla}\times\mathbf{B}(x)-\dot{\mathbf{E}}(x) &= \boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{A}(x)-\dot{\mathbf{E}}(x)\\ &= -\left[\boldsymbol{\nabla}^2\mathbf{A}(x)-\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\mathbf{A}(x)\right]-\dot{\mathbf{E}}(x)=\frac{1}{c}\mathbf{j}(x).\end{aligned} \tag{10.11}$$

If the electron moves along a trajectory $\mathbf{x}(t)$, the potential energy becomes

$$V(t)=e\phi\left(\mathbf{x}(t),t\right). \tag{10.12}$$

In the Lagrangian $L=T-V$ this contributes with the opposite sign

$$L^{\rm int}(t)=-eA^0\left(\mathbf{x}(t),t\right) \tag{10.13}$$

giving a potential part of the interaction

$$\mathcal{A}^{\rm int}\big|_{\rm pot}=-e\int dtA^0\left(\mathbf{x}(t),t\right). \tag{10.14}$$

Since the time t coincides with $x^0(t)/c$ of the trajectory, this can be expressed as

$$\mathcal{A}^{\rm int}\big|_{\rm pot}=-\frac{e}{c}\int dx^0A^0(x). \tag{10.15}$$

In this form it is now quite simple to write down the complete electromagnetic interaction purely on the basis of relativistic invariance. The minimal invariant extension of (10.16) is obviously

$$\mathcal{A}^{\rm int}=-\frac{e}{c}\int dx^\mu A_\mu(x). \tag{10.16}$$

Thus, the full action of a point particle can be written more explicitly as

$$\begin{aligned}\mathcal{A} &= \int dtL(t)=-mc\int ds-\frac{e}{c}\int dx^\mu A_\mu(x)\\ &= -mc^2\int dt\left[1-\frac{\mathbf{v}^2}{c^2}\right]^{1/2}-e\int dt\left(A^0-\frac{1}{c}\mathbf{v}\cdot\mathbf{A}\right).\end{aligned} \tag{10.17}$$

The canonical formalism supplies the canonically conjugate momenta

$$\mathbf{P}=\frac{\partial L}{\partial\mathbf{v}}=m\frac{\mathbf{v}}{\sqrt{1-\mathbf{v}^2/c^2}}+\frac{e}{c}\mathbf{A}\equiv\mathbf{p}+\frac{e}{c}\mathbf{A}. \tag{10.18}$$

Thus the velocity is related to the canonical momenta and external field via

$$\frac{\mathbf{v}}{c} = \frac{\mathbf{P} - \frac{e}{c}\mathbf{A}}{\sqrt{\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + m^2c^2}}. \tag{10.19}$$

This can be used to calculate the Hamiltonian via the Legendre transform

$$H = \frac{\partial L}{\partial \mathbf{v}}\mathbf{v} - L = \mathbf{P} \cdot \mathbf{v} - L \tag{10.20}$$

giving

$$H = c\sqrt{\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + m^2c^2} + eA^0. \tag{10.21}$$

In the non-relativistic limit this has the expansion

$$H = mc^2 + \frac{1}{2m}\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + eA^0 + \dots \tag{10.22}$$

Thus the free theory goes over into the interacting theory by what is called the *minimal substitution* law

$$\begin{aligned} \mathbf{p} &\longrightarrow \mathbf{p} - \frac{e}{c}\mathbf{A} \\ H &\longrightarrow H - eA^0 \end{aligned} \tag{10.23}$$

or, in relativistic notation,

$$p^\mu \longrightarrow p^\mu - \frac{e}{c}A^\mu. \tag{10.24}$$

10.1.2 Electrodynamics and Quantum Mechanics

When going over from quantum mechanics to second quantized field theories we found the rule that a non-relativistic Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \tag{10.25}$$

became an operator

$$H = \int d^3x \psi^\dagger(\mathbf{x}, t)\left[-\frac{\boldsymbol{\nabla}^2}{2m} + V(\mathbf{x})\right]\psi(\mathbf{x}, t), \tag{10.26}$$

where we have omitted the operator hats, for brevity. With the same rules we see that the second quantized form of the interacting nonrelativistic Hamiltonian in a static $A(\mathbf{x})$ field,

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + eA^0, \tag{10.27}$$

is given by

$$H=\int d^3x\,\psi^\dagger(\mathbf{x},t)\left[-\frac{1}{2m}\left(\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A}\right)^2+eA^0\right]\psi(\mathbf{x},t). \tag{10.28}$$

When going to the action of this theory we find

$$\begin{aligned}\mathcal{A}=\int dtL=\int dt\int d^3x\,\Big[&\psi^\dagger(\mathbf{x},t)\left(i\partial_t+eA^0\right)\psi(\mathbf{x},t)\\ &+\frac{1}{2m}\psi^\dagger(\mathbf{x},t)\left(\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A}\right)^2\psi(\mathbf{x},t)\Big].\end{aligned} \tag{10.29}$$

It is easy to verify that (10.28) reemerges from the Legendre transform

$$H=\frac{\partial L}{\partial\dot\psi(\mathbf{x},t)}\dot\psi(\mathbf{x},t)-L. \tag{10.30}$$

The action (10.29) holds also for time-dependent $A^\mu(x)$ fields.

We can now deduce the second quantized form of the minimal substitution law (10.23) which is

$$\begin{aligned}\boldsymbol{\nabla}&\rightarrow\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A}(\mathbf{x},t),\\ \partial_t&\rightarrow\partial_t+ieA^0(\mathbf{x},t),\end{aligned} \tag{10.31}$$

or covariantly:

$$\partial_\mu\rightarrow\partial_\mu-i\frac{e}{c}A_\mu(x). \tag{10.32}$$

This substitution rule has the important property that the gauge invariance of the free photon action is preserved by the interacting theory: If we perform the gauge transformation

$$A^\mu(x)\rightarrow A^\mu(x)+\partial^\mu\Lambda(x), \tag{10.33}$$

i.e.,

$$\begin{aligned}A^0(\mathbf{x},t)&\rightarrow A^0(\mathbf{x},t)+\partial_t\Lambda(\mathbf{x},t)\\ \mathbf{A}(\mathbf{x},t)&\rightarrow\mathbf{A}(\mathbf{x},t)-\boldsymbol{\nabla}\Lambda(\mathbf{x},t),\end{aligned} \tag{10.34}$$

the action remains invariant if we simultaneously change the fields $\psi(\mathbf{x},t)$ of the charged particles by a spacetime-dependent phase

$$\psi\,(\mathbf{x},t)\rightarrow e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\psi(\mathbf{x},t). \tag{10.35}$$

Under this transformation, the derivatives of the field change like

$$\begin{aligned}\boldsymbol{\nabla}\psi(\mathbf{x},t)&\rightarrow e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left[\boldsymbol{\nabla}-i\frac{e}{c}\boldsymbol{\nabla}\Lambda(\mathbf{x},t)\right]\psi,\\ \partial_t\psi&\rightarrow e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left(\partial_t-ie\partial_t\Lambda\right)\psi(\mathbf{x},t).\end{aligned} \tag{10.36}$$

The modified derivatives appearing in the action have therefore the following simple transformation law:

$$\begin{aligned} \left(\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A}\right)\psi(\mathbf{x},t) &\rightarrow e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left(\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A}\right)\psi(\mathbf{x},t), \\ \left(\partial_t+i\frac{e}{c}A^0\right)\psi(\mathbf{x},t) &\rightarrow e^{-i\frac{e}{c}\Lambda(\mathbf{x},t)}\left(\partial_t+ieA^0\right)\psi(\mathbf{x},t). \end{aligned} \tag{10.37}$$

These combinations of derivatives and gauge fields are called *covariant derivatives* and written as

$$\begin{aligned} \mathbf{D}\psi(\mathbf{x},t) &\equiv \left(\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A}\right)\psi(\mathbf{x},t) \\ D_t\psi(\mathbf{x},t) &\equiv \left(\partial_t+ieA^0\right)\psi(\mathbf{x},t) \end{aligned} \tag{10.38}$$

or, in four-vector notation,

$$D_\mu\psi(x) = \left(\partial_\mu+i\frac{e}{c}A_\mu\right)\psi(x). \tag{10.39}$$

Here the adjective covariant does not refer to the Lorentz group but to the gauge group. It records the fact that $D_\mu\psi$ transforms under local gauge changes (10.31) of ψ in the same way as ψ itself in (10.35):

$$D_\mu\psi(x) \rightarrow e^{-i\frac{e}{c}\Lambda(x)}D_\mu\psi(x). \tag{10.40}$$

With the help of this covariant derivative any action which is invariant under global phase changes [i.e., $U(1)$-invariant in the sense discussed in Chapter 4] by a constant phase angle

$$\psi(x) \rightarrow e^{-i\alpha}\psi(x) \tag{10.41}$$

can easily be made invariant under local gauge transformations (10.33). We merely have to replace all derivatives by covariant derivatives (10.39) and adding the gauge invariant photon Lagrangian (10.3).

10.1.3 Electrodynamics and Relativistic Quantum Mechanics

Let us follow this rule for relativistic electrons and replace, in the Lagrangian (10.2),

$$\partial\!\!\!/ = \gamma^\mu\partial_\mu \rightarrow \gamma^\mu\left(\partial_\mu+i\frac{e}{c}A_\mu\right) = \left(\partial\!\!\!/+i\frac{e}{c}A\!\!\!/\right) \equiv D\!\!\!\!/\,. \tag{10.42}$$

In this way we arrive at the Lagrangian of quantum electrodynamics (QED)

$$\mathcal{L}(x) = \bar\psi(x)\left(iD\!\!\!\!/-m\right)\psi(x) - \frac{1}{4}F_{\mu\nu}^2. \tag{10.43}$$

The classical field equations can easily be found by extremizing the action and variation with respect to all fields which gives

$$\frac{\delta\mathcal{A}}{\delta\bar\psi(x)} = (i\not\partial - m)\,\psi(x) = 0 \tag{10.44}$$

$$\frac{\delta\mathcal{A}}{\delta A_\mu(x)} = \partial_\nu F^{\nu\mu}(x) - \frac{1}{c}j^\mu(x) = 0. \tag{10.45}$$

with the *current density*

$$j^\mu(x) \equiv ec\bar\psi(x)\gamma^\mu\psi(x). \tag{10.46}$$

Equation (10.45) coincides Maxwell equation for the electromagnetic field around a classical four-dimensional vector current $j^\mu(x)$:

$$\partial_\nu F^{\nu\mu}(x) = \frac{1}{c}j^\mu(x). \tag{10.47}$$

In the Lorentz gauge $\partial_\mu A^\mu(x) = 0$, this equation reads simply

$$-\,\partial^2 A^\mu(x) = \frac{1}{c}j^\mu(x). \tag{10.48}$$

The current j^μ combines the charge density $\rho(x)$ and the current density $\mathbf{j}$ of particles of charge e in a four-vector

$$j^\mu = (c\rho, \mathbf{j})\,. \tag{10.49}$$

In terms of electric and magnetic fields $E^i = F^{i0}$, $B^i = -F^{jk}$, the field equations (10.47) turn into the Maxwell equations

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{E} &= \rho = e\bar\psi\gamma^0\psi = e\psi^\dagger\psi \\ \boldsymbol{\nabla}\times\mathbf{B} - \dot{\mathbf{E}} &= \frac{1}{c}\mathbf{j} = \frac{e}{c}\bar\psi\boldsymbol{\gamma}\psi. \end{aligned} \tag{10.50}$$

The first is Coulomb's law, the second Ampere's law in the presence of charges and currents.

Note that the physical units employed here differ from those used in many books of classical electrodynamics [1] by the absence of a factor $1/4\pi$ on the right-hand side. The Lagrangian used in those books is

$$\begin{aligned} \mathcal{L}(x) &= -\frac{1}{8\pi}F^2_{\mu\nu}(x) - \frac{1}{c}j^\mu(x)A_\mu(x) \\ &= \frac{1}{4\pi}\left[\mathbf{E}^2(x) - \mathbf{B}^2(x)\right] - \left[\rho(x)\phi(x) - \frac{1}{c}\mathbf{j}(x)\cdot\mathbf{A}(x)\right], \end{aligned} \tag{10.51}$$

which leads to Maxwell's field equations

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{E} &= 4\pi\rho, \\ \boldsymbol{\nabla}\times\mathbf{B} &= \frac{4\pi}{c}\mathbf{j}. \end{aligned} \tag{10.52}$$

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[1] See for example J. D. Jackson, *Classical Electrodynamics*, Wiley and Sons, New York, 1967.

The form employed conventionally in quantum field theory arises from this by replacing $A \to \sqrt{4\pi}A$ and $e \to \sqrt{4\pi}e$. The charge of the electron in our units has therefore the numerical value

$$e = -\sqrt{4\pi\alpha} \approx -\sqrt{4\pi/137} \tag{10.53}$$

rather than $e = -\sqrt{\alpha}$.

10.2 Noether's Theorem and Gauge Fields

In electrodynamics, the conserved charge resulting from the U(1)-symmetry of the matter Lagrangian is the source of a massless particle, the photon. This is described by a gauge field which is minimally coupled to the conserved current. A similar structure will be seen to exists for many internal symmetries giving rise to nonabelian versions of the photon, such as gluons which are the origin of strong interactions, and W- and Z-vector mesons, which mediate the weak interactions.

It is useful to reconsider Noether's derivation of conservation laws in such theories.

The conserved matter current in a locally gauge invariant theory cannot be found any more by the rule (6.114) which was so useful in the globally invariant theory. Here it would read

$$j_\mu = \frac{\delta \mathcal{L}^\epsilon}{\partial \partial_\mu \Lambda}. \tag{10.54}$$

and yield identically zero. We may, however, subject *just* the matter field to a local gauge transformation at *fixed* gauge fields. Then we obtain the correct current

$$j_\mu \equiv \left.\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \Lambda}\right|_{\rm ph}. \tag{10.55}$$

Since the complete change under local gauge transformations $\delta_{\rm s}^x \mathcal{L}$ vanishes identically, we can alternatively vary *only* the gauge fields and keep the matter field fixed

$$j_\mu = -\left.\frac{\partial \mathcal{L}^\epsilon}{\partial \partial_\mu \Lambda}\right|_{\rm m}. \tag{10.56}$$

This is done most simply by forming the functional derivative with respect to the gauge field and omitting the contribution of $\overset{\rm ph}{\mathcal{L}}$:

$$j_\mu = -\frac{\partial \overset{\rm m}{\mathcal{L}}{}^\epsilon}{\partial \partial_\mu \Lambda}. \tag{10.57}$$

Note that if we form the variation of the gauge field action

$$\delta_{\rm s} \overset{\rm ph}{\mathcal{A}} = \int d^4x \; {\rm tr} \left[\delta_{\rm s}^x A_\mu \frac{\delta \overset{\rm ph}{\mathcal{A}}{}^\epsilon}{\delta A_\mu} \right] \tag{10.58}$$

and insert for $\delta_s^x A$ an infinitesimal pure gauge field configuration

$$\delta_s^x A_\mu = -i\partial_\mu \Lambda(x) \tag{10.59}$$

the right-hand side must vanish for all $\Lambda(x)$. After a partial integration this implies the local conservation law $\partial_\mu j^\mu(x) = 0$ for the current

$$j^\mu(x) = -i\frac{\delta \overset{\text{ph}}{\mathcal{A}}}{\delta A_\mu}. \tag{10.60}$$

In contrast to the earlier conservation laws derived for matter fields which were valid only if the matter fields obey the Euler-Lagrange equations, the current conservation law for gauge fields is valid for *all* field configurations. It is an *identity*. In fact, using the Lagrangian (10.3) we find from (10.60) conserved current $j^\nu = \partial_\mu F_{\mu\nu}/2$, which is trivially conserved, due to the asymmetry of $F_{\mu\nu}$.

10.3 Quantization

The canonical formalism can be used to identify canonical momenta

$$\pi_\psi(x) = \frac{\partial \mathcal{L}}{\partial \psi(x)} = \psi^\dagger(x) \tag{10.61}$$

and

$$\pi_{A^i}(x) \equiv \pi^i(x) = F^{0i}(x) = -E^i(x) \tag{10.62}$$

and to find the Hamiltonian density

$$\begin{aligned} \mathcal{H}(x) &= \frac{\partial L}{\partial \dot{\psi}(x)}\dot{\psi}(x) + \frac{\partial \mathcal{L}(x)}{\partial \dot{A}^k(x)} - \mathcal{L}(x) \\ &= \bar{\psi}(-i\boldsymbol{\gamma}\boldsymbol{\nabla} + m)\psi + \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2) + \boldsymbol{\nabla}A^0 \cdot \mathbf{E} + e\bar{\psi}\gamma_\mu\psi A^\mu. \end{aligned} \tag{10.63}$$

Here and in all the subsequent discussion we use natural units in which the light velocity is equal to unity.

The quantization procedure in the presence of interactions now goes as follows: The Dirac field of the electron has the same equal-time anticommutation rules as in the free case:

$$\begin{aligned} \{\psi_a(\mathbf{x},t), \psi_b^\dagger(\mathbf{x}',t)\} &= \delta^{(3)}(\mathbf{x}'-\mathbf{x})\delta_{ab}, \\ \{\psi(\mathbf{x},t), \psi(\mathbf{x}',t)\} &= 0, \\ \{\psi^\dagger(\mathbf{x},t)\psi^\dagger(x't)\} &= 0. \end{aligned} \tag{10.64}$$

For the photon field we first write down the naive commutation rules of the spatial components:

$$\begin{aligned} -\left[E_i(\mathbf{x},t), A_j(\mathbf{x}',t)\right] &= -i\delta^{(3)}(\mathbf{x}-\mathbf{x}')\delta_{ij} && (10.65)\\ \left[A_i(\mathbf{x},t), A_j(\mathbf{x}',t)\right] &= 0, && (10.66)\\ \left[E_i(\mathbf{x},t), E_j(\mathbf{x}',t)\right] &= 0. \end{aligned}$$

As in Subsec. 5.3.1, the first commutator cannot be true here, since by Coulomb's law (10.50),

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{E} &= -\boldsymbol{\nabla}\cdot\dot{\mathbf{A}} - \boldsymbol{\nabla}^2 A^0 \\ &= e\psi^\dagger\psi, && (10.67) \end{aligned}$$

and we want the canonical fields A_i to be independent of ψ and commute with them. The contradiction can be removed just as in the free case by postulating (10.65) only for the transverse parts of E_i and using $\delta^T_{ij}(\mathbf{x}-\mathbf{x}')$ as in (5.333) while letting the longitudinal part $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)$ be a c-number field, since it commutes with all $A^i(\mathbf{x},t)$. The correct commutation rules are the following:

$$\begin{aligned} \left[\dot{A}_j(\mathbf{x},t), A_j(\mathbf{x}',t)\right] &= -i\delta^T_{ij}(\mathbf{x}-\mathbf{x}'),\\ \left[A_j(\mathbf{x},t), A_j(\mathbf{x}',t)\right] &= 0, && (10.68)\\ \left[\dot{A}_i(\mathbf{x},t), \dot{A}_j(\mathbf{x}',t)\right] &= 0. \end{aligned}$$

To calculate the temporal behavior of an arbitrary observable composed of ψ, $\psi^\dagger$ and $A_i, \dot{A}_i$ fields, only one more set of commutation rules has to be specified which are those with A^0. This occurs in the Hamiltonian density (10.63) and is not a canonical variable. In contrast to the free-field case in Section 5.3 it is no longer a c-number. To see this we have to express A^0 in terms of the dynamical fields using Coulomb's law (10.67):

$$A^0(\mathbf{x},t) = \frac{1}{4\pi}\int d^3x' \frac{1}{|\mathbf{x}'-\mathbf{x}|}\left(e\psi^\dagger\psi + \boldsymbol{\nabla}\cdot\dot{\mathbf{A}}\right)(\mathbf{x}',t). \qquad (10.69)$$

This replaces Eq. (3.258) in the presence of charges. In an infinite volume with asymptotically vanishing fields there is no freedom of adding a solution of the homogenous Poisson equation (3.259). While $\boldsymbol{\nabla}\cdot\mathbf{A}$ is a c-number field, the time component of the gauge field A^0 is now a non-local operator involving the fermion field. With these fields being independent of the electromagnetic field, A^0 still commutes with the canonical A_i, $\dot{A}_j$ fields:

$$\left[A^0(\mathbf{x},t), A^i(\mathbf{x}')\right] = \left[A^0(\mathbf{x},t), \dot{A}^i(\mathbf{x}',t)\right] = 0. \qquad (10.70)$$

The commutator with the Fermi fields, on the other hand, is nonzero:

$$\left[A^0(\mathbf{x},t), \psi(\mathbf{x}',t)\right] = -\frac{e}{4\pi|\mathbf{x}-\mathbf{x}'|}\psi(\mathbf{x},t). \qquad (10.71)$$

Note the peculiar property of A^0: It does not commute with the electron field no matter how large the distance between the space points is. This property is called *non-locality*. It is a typical property of the present transverse covariant quantization procedure.

Certainly, the arbitrary c-number function $\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x},t)$ can be made zero by an appropriate gauge transformation as in (3.247).

In the Hamiltonian, the field A^0 can be completely removed by a partial integration:

$$\int d^3x \boldsymbol{\nabla} A^0 \cdot \mathbf{E} = -\int d^3x A^0 \boldsymbol{\nabla}\cdot\mathbf{E}, \tag{10.72}$$

setting the surface term equal to zero, and using the field equation

$$\boldsymbol{\nabla}\cdot\mathbf{E} = e\psi^\dagger\psi. \tag{10.73}$$

Then

$$\begin{aligned} H &= \int d^3x \mathcal{H} \qquad (10.74)\\ &= \int d^3x \left\{\bar\psi\left[-i\boldsymbol{\gamma}\cdot(\boldsymbol{\nabla}-i\frac{e}{c}\mathbf{A})+m\right]\psi+\frac{1}{2}\left(\mathbf{E}^2+\mathbf{B}^2\right)\right\}. \end{aligned}$$

When looking at this expression, one may wonder where the electrostatic interaction has gone. The answer is found by decomposing the electric field

$$E^i = -\partial^0 A^i + \partial^i A^0 \tag{10.75}$$

into longitudinal and transverse parts E^i_L and E^i_T with $\mathbf{E}_L\cdot\mathbf{E}_T = 0$:

$$\begin{aligned} E^i_L &= \partial^i\left(A^0 - \frac{\partial^i\partial^i}{\boldsymbol{\nabla}^2}A^j\right),\\ E^i_T &= -\partial^0\left(\delta^{ij}-\frac{\partial^i\partial^j}{\boldsymbol{\nabla}^2}\right)A^j. \end{aligned} \tag{10.76}$$

Then the field energy becomes

$$\frac{1}{2}\int d^3x\left(\mathbf{E}^2+\mathbf{B}^2\right) = \frac{1}{2}\int d^3x\left(\mathbf{E}_T^2+\mathbf{B}^2\right)+\frac{1}{2}\int d^3x\mathbf{E}_L^2. \tag{10.77}$$

Using (10.69) we see that the longitudinal field is simply given by

$$\begin{aligned} \mathbf{E}_L(x) &= -\frac{1}{4\pi}\boldsymbol{\nabla}\int d^3x'\frac{1}{|\mathbf{x}-\mathbf{x}'|}e\psi^\dagger(\mathbf{x}',t)\psi(\mathbf{x}',t)\\ &= \boldsymbol{\nabla}\left[\frac{1}{\boldsymbol{\nabla}^2}e\psi^\dagger(x)\psi(x)\right]. \end{aligned} \tag{10.78}$$

This is the Coulomb field caused by the charge density of the electron $e\psi^\dagger(x)\psi(x)$. The field energy carried by $E_L^i(x)$ is

$$\begin{aligned}\frac{1}{2}\int d^3x\,\mathbf{E}_L^2(x) &= \frac{e^2}{2}\int d^3x\left\{\boldsymbol{\nabla}\left[\frac{1}{\boldsymbol{\nabla}^2}\psi^\dagger(x)\psi(x)\right]\right\}^2\\ &= -\frac{e^2}{2}\int d^3x\,\psi^\dagger(x)\psi(x)\frac{1}{\boldsymbol{\nabla}^2}\psi^\dagger(x)\psi(x)\\ &= \frac{e^2}{8\pi}\int d^3xd^3x'\,\psi^\dagger(\mathbf{x},t)\psi(\mathbf{x},t)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\psi^\dagger(\mathbf{x}',t)\psi(\mathbf{x}',t),\end{aligned} \tag{10.79}$$

and coincides precisely with the Coulomb energy associated with the charge density (10.50).

The term $\frac{1}{2}\int d^3x\left(\mathbf{E}_T^2+\mathbf{B}^2\right)$ in Eq. (10.77) is an operator and contains the energy of the field quanta.

In order to develop a perturbation theory for QED in this quantization, we must specify the free and interacting parts of the action. Since A^0 and $\boldsymbol{\nabla}\cdot\mathbf{A}$ are unquantized and appear only quadratically in the action, they may be eliminated in the same way as in the energy and lead to the action

$$\mathcal{A}=\int d^4x\left\{\bar\psi(x)(i\partial\!\!\!/-M)\psi(x)+\frac{1}{2}\left[\mathbf{E}_T^2(x)-\mathbf{B}^2(x)\right]\right\}+\mathcal{A}^{\rm int}, \tag{10.80}$$

where the first two terms are the actions of the quantized Dirac and transverse electromagnetic fields ψ and $\mathbf{A}_T$, and $\mathcal{A}^{\rm int}$ is the interaction

$$\mathcal{A}^{\rm int}=-\frac{e^2}{8\pi}\int dt\int d^3xd^3x'\psi^\dagger(\mathbf{x},t)\psi(\mathbf{x},t)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\psi(\mathbf{x}',t)\psi(\mathbf{x}',t)+\int d^4x\frac{1}{c}\mathbf{j}\cdot\mathbf{A}_T. \tag{10.81}$$

The interaction contains two completely different terms: The first is an instantaneous Coulomb interaction at a distance which takes place without retardation and involves four Dirac fields. It is nontrivial to show that this does not cause any conflicts with relativity.

The special role of the Coulomb interaction is avoided by the Gupta-Bleuler quantization procedure. Here the free action is

$$\mathcal{A}=\int d^4x\left[\bar\psi\left(i\partial\!\!\!/-m\right)\psi-\frac{1}{4}F^{\mu\nu}F_{\mu\nu}-D\partial^\mu A_\mu+D^2/2\right], \tag{10.82}$$

and the interaction has the manifestly covariant form

$$\mathcal{A}^{\rm int}=-\int d^4xj^\mu A_\mu. \tag{10.83}$$

10.4 Perturbation Theory

It is easy to set up the Feynman diagrams. The free-particle propagators of the electrons was given in (5.276). Since we want to calculate the effect of interactions, we shall from now on attach to the free propagator a subscript 0. Thus

$$S_0(x-x') = \int \frac{d^4p}{(2\pi)^4}\frac{i}{\not p - M + i\eta}e^{-ip(x-x')}. \tag{10.84}$$

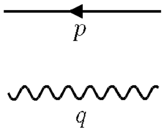
The propagator of the free photon depends on the gauge. It is most simple in the Gupta-Bleuler quantization scheme, where [see (5.495)]

$$G_0^{\mu\nu}(x,x') = -g^{\mu\nu}G_0(x,x') = -g^{\mu\nu}\int \frac{d^4q}{(2\pi)^4}\frac{i}{q^2+i\eta}e^{-ik(x-x')}. \tag{10.85}$$

In a Wick expansion, each contraction is represented by one of these propagators:

$$\begin{aligned} \dot\psi(x)\dot\psi(x') &= S(x-x'), & (10.86)\\ \dot A^\mu(x)\dot A^\nu(x') &= G_0^{\mu\nu}(x-x'). & (10.87) \end{aligned}$$

They are pictured by the lines



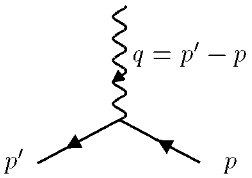
$$= \frac{i}{\not p - m}$$

$$= -g^{\mu\nu}\frac{i}{q^2+i\epsilon}$$

The interaction Lagrangian

$$\mathcal{L}^{\rm int} = -e\bar\psi\gamma^\mu A_\mu(x) \tag{10.88}$$

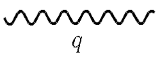
is pictured by the vertex



$$= -e\gamma^\mu. \tag{10.89}$$

With these graphical elements we must form all Feynman diagrams which can contribute to a given physical process.

In the transverse quantization scheme, the Feynman diagrams are much more complicated. Recalling the propagator (5.349), the photon line stands now for

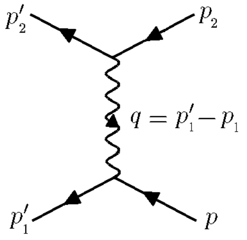


$$= P^{\mu\nu}_{\rm phys}(q)\frac{i}{q^2+i\epsilon}$$

with the physical off-shell polarization sum [recall (10.7)]

$$P^{\mu\nu}_{\rm phys}(q) = -g^{\mu\nu} - \frac{q_\mu q_\nu}{(q\eta)^2 - q^2} + q\eta\frac{q_\mu\eta_\nu + q_\nu\eta_\mu}{(q\eta)^2 - q^2} - \eta_\mu\eta_\nu\frac{q^2}{(q\eta)^2 - q^2}. \tag{10.90}$$

The photon propagator is very complicated due to the appearance of the frame-dependent vector $\eta = (1, 0, 0, 0)$. As a further complication, there are diagrams from the four-fermion Coulomb interactions in (10.81). These can be pictured by

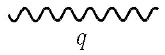


$$= \frac{i}{\mathbf{q}^2}\gamma^0 \times \gamma^0.$$

We now observe that these diagrams may be obtained from an auxiliary interaction

$$\mathcal{A}^{\rm int} = -\int d^4x j^0 A_0 \tag{10.91}$$

assuming the A_0-field to have the propagator



$$= \frac{i}{\mathbf{q}^2}$$

If this propagator is added to the physical one, it cancels precisely the last term in the off-shell polarization sum (10.90), which becomes effectively

$$P^{\mu\nu}_{\rm phys,eff}(\mathbf{k}) = -g^{\mu\nu} - \frac{q_\mu q_\nu}{(q\eta)^2 - q^2} + q\eta\frac{q_\mu\eta_\nu + q_\nu\eta_\mu}{(q\eta)^2 - q^2}. \tag{10.92}$$

Of course, the final physical results cannot depend on the frame in which the theory is quantized. Thus is must be possible to drop all η-dependent terms. We prove this in three steps:

First, a photon may be absorbed (or emitted) by an electron which is on the mass shell before and after the process. The photon propagator is contracted with an electron current as follows

$$\bar{u}(\mathbf{p}', s_3')\gamma_\mu u(\mathbf{p}, s_3')P^{\mu\nu}_{\rm phys,eff}(q). \quad q = p' - p. \tag{10.93}$$

Since the spinors on the right and left-hand side satisfy the Dirac equation, the current is conserved and satisfies

$$\bar{u}(\mathbf{p}', s_3')\gamma_\mu u(\mathbf{p}, s_3')q^\mu = 0. \tag{10.94}$$

This condition eliminates the terms containing the vector q^μ in the polarization sum (10.92). Only the reduced polarization sum

$$P^{\mu\nu}_{\rm red}(q) = -g^{\mu\nu} \tag{10.95}$$

survives, which is the polarization tensor of the Gupta-Bleuler propagator (10.85).

The same elimination happens if a photon is absorbed by an internal line, although due to a slightly more involved mechanism. An internal line may arise in two ways. An electron may enter a Feynman diagram on the mass shell, absorb a number of photons, say n, and leave again on mass shell as shown in Fig. 10.1. The associated off-shell amplitude is

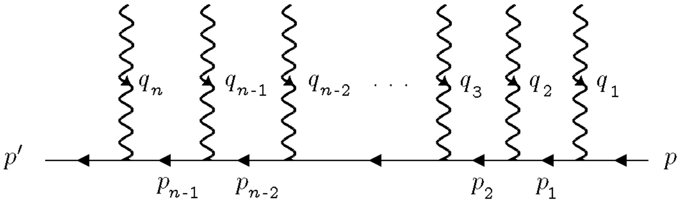


FIGURE 10.1 An electron on the mass shell absorbing several photons and leaving again on the mass shell.

$$a(p',p,q_i) = \frac{1}{\not{p}' - M}\not{q}_n\frac{1}{\not{p}_{n-1} - M}\not{q}_{n-1}\not{q}_{n-1}\cdots\not{q}_3\frac{1}{\not{p}_2 - M}\not{q}_2\frac{1}{\not{p}_1 - M}\not{q}_1. \tag{10.96}$$

It has to be amputated and evaluated between the initial and final spinors, which amounts to multiplying it from the left and right with $\bar{u}(\mathbf{p}',s_3')(\not{p}'-M)$ and $(\not{p}-M)u(\mathbf{p},s_3)$, respectively. If an additional photon is absorbed, it must be inserted $n+1$ times as shown in Fig. 10.2. At each vertex, there is no current conservation since the photon lines are not on mass shell. Nevertheless, the sum of all $n+2$ diagrams does have a conserved current.

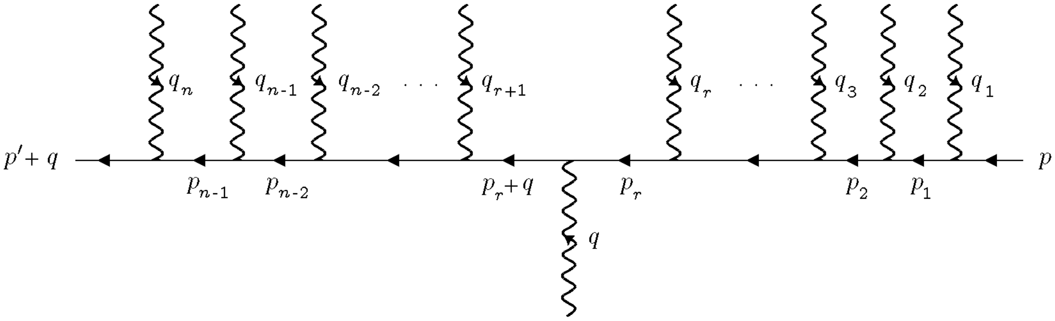


FIGURE 10.2 An electron on the mass shell absorbing several photons, plus an additional photon, and leaving again on the mass shell.

To prove this we observe the following *Ward-Takahashi identity*:

$$\frac{1}{\not{p}_r + \not{q} - M}\not{q}\frac{1}{\not{p}_r - M} = \frac{1}{\not{p}_r - M} - \frac{1}{\not{p}_r + \not{q} - M}. \tag{10.97}$$

The sum of all off-shell absorption diagrams can be written as

$$a(p',p,q_i;q)=\frac{1}{\not p'+\not q-M}\not q_n\frac{1}{\not p_{n-1}+\not q-M}\not q_{n-1}\cdots$$
$$\cdots\frac{1}{\not p_r+\not q-M}\not q\frac{1}{\not p_r-M}\cdots\not q_2\frac{1}{\not p_1-M}\not q_1 u(\mathbf{p},s_3). \quad (10.98)$$

to be evaluated between $\bar u(\mathbf{p}'+\mathbf{q},s_3')(\not p'+\not q-M)$ and $(\not p-M)u(\mathbf{p},s_3)$. With the help of the Ward-Takahashi identity we can now remove the $\not q$ recursively from $a(p',p,q_i;q)$ and remain with the difference

$$a(p',p,q_i;q)=a(p',p,q_i)-a(p'+q,p+q,q_i). \quad (10.99)$$

When evaluating the right-hand side between the above spinors, we see that the first term in the difference vanishes since the left-hand spinor satisfies the Dirac equation. The same thing holds for the second term and the right-hand spinor. Thus the polarization sum in the photon propagator can again be replaced by the reduced expression (10.95).

Finally, the electron line can be a closed to a loop as shown in Fig. 10.3. Here

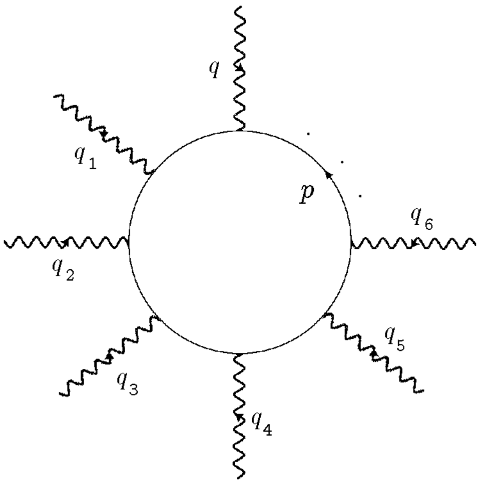


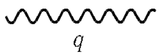
FIGURE 10.3 An internal electron loop absorbing several photons, plus an additional photon, and leaving again on the mass shell.

the amplitude (10.99) appears in a loop integral with an additional photon vertex:

$$\int\frac{d^4p}{(2\pi)^4}\mathrm{tr}\left[\not q\, a(p',p,q_i;q)\right]=\int\frac{d^4p}{(2\pi)^4}\mathrm{tr}\left\{\not q\left[a(p',p,q_i)-a(p'+q,p+q,q_i)\right]\right\}. \quad (10.100)$$

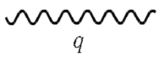
If the divergence of the integral is made finite by a dimensional regularization, the loop integral is translationally invariant in momentum space and the amplitude difference vanishes. Thus, also in this case, the polarization sum can be replaced by the reduced expression (10.95).

Thus we have shown that due to current conservation and the Ward-Takahashi identity, the photon propagator in all Feynman diagrams can be replaced by



$$= G^{\mu\nu}(q) = \frac{-ig^{\mu\nu}}{q^2+i\eta} \tag{10.101}$$

As a matter of fact, for the same reason, any propagator



$$= G^{\mu\nu}(q) = -\frac{i}{q^2}\left[g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}(1-\alpha)\right] \tag{10.102}$$

can just as well be used, for any parameter α. This is the propagators arising when adding to the free Lagrangian the fixing term

$$\mathcal{L}_{\rm GF} = \frac{\alpha}{2}D^2 - D\partial^\mu A_\mu. \tag{10.103}$$

The Feynman value $\alpha = 1$ reduces to (10.101).

10.5 Magnetic Moment of Electron

For dimensional reasons, the magnetic moment of the electron is proportional to the Bohr magnetic moment

$$\mu_{\rm B} = \frac{e^2\hbar}{2Mc}. \tag{10.104}$$

Since it is caused by the spin of the particle, it is proportional to it and can be written as

$$\boldsymbol{\mu} = g\mu_{\rm B}\frac{\mathbf{S}}{\hbar}. \tag{10.105}$$

The proportionality factor g is called the *gyromagnetic ratio*. If the spin is polarized in the z-direction, the z-component of $\boldsymbol{\mu}$ is

$$\mu = g\mu_{\rm B}\frac{1}{2} = g\frac{e^2\hbar}{2Mc}\frac{1}{2}. \tag{10.106}$$

We have discussed in Subsec. 3.16, that as a result of the *Thomas precession* an explanation of the experimental fine structure requires the g-factor of the electron magnetic moment to have the value 2. This is twice as large as that of a charged rotating sphere of angular momentum L, whose magnetic moment is

$$\boldsymbol{\mu} = \frac{e^2\hbar}{2Mc}\frac{\mathbf{L}}{\hbar}, \tag{10.107}$$

i.e., whose g-value is unity. The result $g = 2$ has been found also in Eq. (4.64) by bringing the Dirac equation in an electromagnetic field to the second-order Pauli form (4.55).

Let us convince ourselves that a Dirac particle possesses the correct gyromagnetic ratio $g = 2$. Consider an electron of momentum $\mathbf{p}$ in a electromagnetic field which changes the momentum to $\mathbf{p}'$ (see Fig. 10.89). The interaction Hamiltonian is given by the matrix element

$$H^{\rm int} = \int d^3x A_\mu(\mathbf{x}) \langle \mathbf{p}'|j^\mu(x)|\mathbf{p}\rangle. \tag{10.108}$$

where in Dirac's theory

$$\langle \mathbf{p}', s_3'|j^\mu(x)|\mathbf{p}, s_3\rangle = e\langle 0|a(\mathbf{p}', s_3')\,\bar\psi(x)\gamma^\mu\psi(x)\,a^\dagger(\mathbf{p}, s_3)|0\rangle \tag{10.109}$$

Inserting the field expansion (5.211) in terms of creation and annihilation operators

$$\psi(x) = \sum_{\mathbf{p},s_3} \frac{1}{\sqrt{VE_{\mathbf{p}}/M}} \left[e^{-ipx}u(\mathbf{p}, s_3)a_{\mathbf{p},s_3} + e^{ipx}v(\mathbf{p}, s_3)b^\dagger(\mathbf{p}, s_3)\right], \tag{10.110}$$

and using anticommutators (5.215) and (5.216), we obtain

$$\langle \mathbf{p}', s_3'|j^\mu(x)|\mathbf{p}, s_3\rangle = e\bar u(\mathbf{p}', s_3)\gamma^\mu u(\mathbf{p}, s_3)\frac{e^{i(p'-p)x}}{\sqrt{VE_{\mathbf{p}'}/M}\sqrt{VE_{\mathbf{p}}/M}}. \tag{10.111}$$

The difference between the four-momenta

$$q' \equiv p' - p \tag{10.112}$$

is the *momentum transfer* from the electromagnetic field to the electron.

In order to find the size of the magnetic moment we set up a constant magnetic field in the 3-direction by letting the second component of the vector potential be $A_2(x) = x^1 B_3$. Then we put the final electron to rest, i.e., $p'^\mu = (M, \mathbf{0})$, and let the initial electron move slowly in the 1-direction. We create a spinor $u(\mathbf{p}, s_3)$ by applying a small Lorentz-boost $e^{-i\zeta^1(i\gamma^0\gamma^1)/2}$ to the rest spinors (3.615), and expand the matrix element (10.111) up to the first order in $\mathbf{p}$. To zeroth order, this yields

$$\bar u(\mathbf{0}, s_3')\gamma^\mu u(\mathbf{0}, s_3) = \chi^\dagger(s_3')\chi(s_3)\delta^\mu{}_0 \tag{10.113}$$

showing that the charge is unity. The linear term in q^1 gives rise to a 2-component:

$$\langle \mathbf{p}', s_3'|j^2(x)|\mathbf{p}, s_3\rangle = e\bar u(\mathbf{0}, s_3)\gamma^2 e^{-i\zeta^1(i\gamma^0\gamma^1)/2}u(\mathbf{0}, s_3)\frac{e^{iq^1x^1}}{V}. \tag{10.114}$$

The two normalization factors on the right-hand side of (10.111) differ only by second-order terms in q^1, Now, since $\bar u(\mathbf{0}, s_3)\gamma^2 u(\mathbf{0}, s_3) = 0$ and $i\gamma^1\gamma^2/2 = S_3$, the spinors on the right-hand side reduce to

$$-ie\zeta^1 u^\dagger(\mathbf{0}, s_3)S_3 u(\mathbf{0}, s_3) = -ie\zeta^1 s_3. \tag{10.115}$$

Momentum conservation enforces $\zeta^1 = -q^1/M$, so that we find

$$\langle \mathbf{p}', s_3' | j^2(x) | \mathbf{p}, s_3 \rangle = ie\frac{q^1}{M}s_3\frac{e^{iq^1x^1}}{V}. \tag{10.116}$$

Inserting this into the interaction Hamiltonian (10.108), we obtain

$$\begin{aligned} E^{\rm int} &= \lim_{q^1\to 0}\int d^3x A_2(\mathbf{x}) iq^1 e^{iq^1x^1}\frac{e}{M}s_3\frac{1}{V} = \lim_{q^1\to 0}\int d^3x\, A_2(\mathbf{x})\partial_1 e^{iq^1x^1}\frac{e}{M}s_3\frac{1}{V} \\ &= -\int d^3x\,\partial_1 A_2(\mathbf{x})\frac{e}{M}s_3\frac{1}{V} \end{aligned} \tag{10.117}$$

Inserting now the vector potential $A_2(x) = x^1B_3$ yields the magnetic interaction Hamiltonian

$$H^{\rm int} = -B_3\frac{e}{M}s_3. \tag{10.118}$$

Since a magnetic moment μ interacts with a magnetic field with the energy $-\boldsymbol{\mu}\mathbf{B}$, we read off the magnetic moment (10.106), implying a gyromagnetic ratio $g = 2$.

Note that the magnetic field caused by the orbital motion of an electron leads to a coupling of the orbital angular momentum $\mathbf{L} = \mathbf{x}\times\mathbf{p}$ with a g-factor $g = 1$. In order to see this relative factor 2 most clearly, consider the intraction Hamiltonian

$$H^{\rm int} = -\int d^3x \mathbf{A}(x)\langle \mathbf{p}', s_3' | \mathbf{j}(x) | \mathbf{p}, s_3\rangle, \tag{10.119}$$

and insert the Dirac current (10.111). For slow electrons we may neglect quantities of second order in the momenta, so that the normalization factors E/M are unity, and obtain

$$H^{\rm int} = -e\int d^3x\, \mathbf{A}(x)\bar u(\mathbf{p}', s_3)\boldsymbol{\gamma}\, u(\mathbf{p}, s_3)e^{-i(\mathbf{p}'-\mathbf{p})\mathbf{x}} \tag{10.120}$$

At this place we make use of the so-called *Gordon decomposition formula*

$$\bar u(\mathbf{p}', s_3')\gamma^\mu u(\mathbf{p}, s_3) = \bar u(\mathbf{p}', s_3')\left[\frac{1}{2M}(p'^\mu + p^\mu) + \frac{i}{2M}\sigma^{\mu\nu}q_\nu\right]u(\mathbf{p}, s_3), \tag{10.121}$$

where $q \equiv p' - p$ is the momentum transfer. This formula follows directly from the anticommutation rules of the γ-matrices and the Dirac equation.

An alternative decomposition is

$$\langle \mathbf{p}' | j^\mu | \mathbf{p}\rangle = e\bar u(\mathbf{p}')\left[\frac{1}{2M}(p'^\mu + p^\mu)F_1(q^2) + \frac{i}{2M}\sigma^{\mu\nu}q_\nu F_2(q^2)\right]u(\mathbf{p}'), \tag{10.122}$$

with the form factors $F_1(q^2)$, $F_2(q^2)$ related to $F(q^2)$, $G(q^2)$ via (10.121) by

$$F(q^2) = F_1(q^2), \qquad G(q^2) = F_1(q^2) + F_2(q^2). \tag{10.123}$$

Then we rewrite the interaction Hamiltonian as

$$H^{\rm int} = -\frac{e}{M}\int d^3x \mathbf{A}(x)\,\bar u(\mathbf{p}', s_3)\,(\mathbf{p} + \mathbf{q} - i\mathbf{q}\times\mathbf{S})\,u(\mathbf{p}, s_3)e^{-i\mathbf{q}\mathbf{x}}, \tag{10.124}$$

where we have used the relations (3.472) and (3.469). We now replace $\mathbf{q}$ by the derivatives $i\partial_{\mathbf{x}}$ in front of the exponential $e^{-i\mathbf{qx}}$, and perform an integration by parts to make the derivatives act on the vector potential $\mathbf{A}(x)$, with the opposite sign. In the transverse gauge, the term $\mathbf{A}(x)\cdot\mathbf{q}$ gives zero while $-i\mathbf{A}(x)\cdot(\mathbf{q}\times\mathbf{S})$ becomes $\mathbf{B}\cdot\mathbf{S}$. For equal incoming and outgoing momenta, this leads to the interaction Hamiltonian

$$H^{\rm int}=-\frac{e}{M}\int d^3x\,[\mathbf{A}(x)\cdot\mathbf{p}+\mathbf{B}(x)\cdot\mathbf{S}] \tag{10.125}$$

We now express the vector potential in terms of the magnetic field as

$$\mathbf{A}(x)=\frac{1}{2}\mathbf{B}\times\mathbf{x}, \tag{10.126}$$

and rewrite (10.125) in the final form

$$H^{\rm int}=-\frac{e}{2M}\mathbf{B}\cdot(\mathbf{L}+2\mathbf{S}), \tag{10.127}$$

where $\mathbf{L}=\mathbf{x}\times\mathbf{p}$ is the with orbital angular momentum. The relative factor 2 between orbital and spin angular momentum gives rise to a characteristic splitting of atomic energy levels in an external magnetic field. If the field is weak, we rewrite $\mathbf{L}+2\mathbf{S}$ as $\mathbf{J}+\mathbf{S}$. For a weak external field the spin will orient itself on the average in the direction of the total angular momentum, i.e.,

$$\bar{\mathbf{S}}=\mathbf{J}\frac{\mathbf{J}\cdot\mathbf{S}}{\mathbf{J}^2}. \tag{10.128}$$

By rewriting

$$\mathbf{J}\cdot\mathbf{S}=\frac{1}{2}\left(\mathbf{J}^2+\mathbf{S}^2-\mathbf{L}^2\right), \tag{10.129}$$

we see that

$$\bar{\mathbf{S}}=f\,\mathbf{J} \tag{10.130}$$

with a factor

$$f=\left[J(J+1)+S(S+1)-L(L+1)\right]/2J(J+1). \tag{10.131}$$

Inserting this into (10.127), we obtain the interaction energies of an atomic state $|JM\rangle$:

$$H^{\rm int}=-\frac{e}{2M}BMg,\qquad g=1+f. \tag{10.132}$$

This typical gyromagnetic ratio has been observed in many experiments.

10.6 Decay of Atomic State

The first important result of quantum electrodynamics is the explanation of the decay of an atom. In quantum mechanics, this decay can only be studied by means of the correspondence principle.

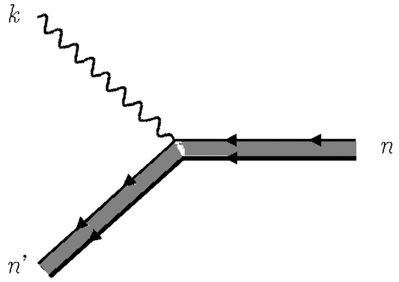


FIGURE 10.4 Transition of an atomic state from a state n with energy E_n to a lower state n' with energy $E_{n'}$, thereby emitting a photon with a frequency $\omega = (E_{n'} - E_n)/\hbar$

Consider an electron in an atomic state undergoing a transition from a state n with energy E_n to a lower state n' with energy $E_{n'}$, whereby a photon is emitted with a frequency $\omega = (E_{n'} - E_n)/\hbar$ (see Fig. 10.4). Following the correspondence principle one imagines the center of gravity of the electronic cloud to oscillate with this frequency with an amplitude

$$\mathbf{x}_0 = \sum_\nu \langle n'|\mathbf{x}^{(\nu)}|n\rangle, \tag{10.133}$$

where the sum runs over all electron coordinates. The oscillating charge emits antenna radiation.

Let us recall the power emitted by an accelerated charge. It is associated with a current

$$j^\mu(x) = e\int d\tau\, \dot{x}^\mu(\tau)\, \delta^{(4)}(\mathbf{x} - \bar{\mathbf{x}}(\tau)). \tag{10.134}$$

To find the electromagnetic field emerging from this we solve the field equation in the Lorentz gauge $\partial_\mu A^\mu = 0$ [recall (10.48)]

$$\partial^2 A^\mu(x) = \frac{1}{c} j^\mu(y), \tag{10.135}$$

by [compare (5.180) and (5.181)]

$$A^\mu(x) = \frac{i}{c}\int d^4y\, G_R(x-y)\, j^\mu(y), \tag{10.136}$$

where $G^R(x-y)$ is the retarded Green function (5.171):

$$G_R(x-x') = -i\Theta(x^0 - x'^0)\frac{1}{4\pi R}\left[\delta(x^0 - x'^0 - R) - \delta(-x^0 + x'^0 + R)\right]. \tag{10.137}$$

By comparison with (5A.8) we see that the result is the Linard-Wiechert potential:

$$A^0(x) = \frac{1}{4\pi}\left[\frac{e}{(1-\mathbf{n}\cdot\bar{\mathbf{v}}/c)R}\right]_{\rm ret}, \qquad \mathbf{A}(x) = \frac{1}{4\pi}\left[\frac{e\bar{\mathbf{v}}/c}{(1-\mathbf{n}\cdot\bar{\mathbf{v}}/c)R}\right]_{\rm ret}. \tag{10.138}$$

where

$$\bar{\mathbf{v}}(t) \equiv \dot{\bar{\mathbf{x}}}(t) \tag{10.139}$$

is the velocity along the trajectory $\bar{\mathbf{x}}(t)$,

$$\mathbf{R}(t) = \mathbf{x} - \bar{\mathbf{x}}(t). \tag{10.140}$$

is the distance vector from the charge, and

$$\mathbf{n}(t) \equiv \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|} \tag{10.141}$$

is the direction of the distance vector. The brackets with the subscript "ret" indicate that the time argument is retarded with respect to the time on the left-hand side of the equation [recall (5A.5)]:

$$t \to t_R \equiv t - R(t_R)/c. \tag{10.142}$$

Note that the factor $1/\gamma$ in the similar Linard-Wiechert potential (5A.8) for a scalar field is canceled here by extra the relativistic velocity factor $\dot{x}^0(\tau)$ in the zeroth component of the current (10.134) in comparison with the scalar current (5A.1). Also in contrast to (5A.8), we have kept the light velocity c explicitly in the expressions. By forming the combinations (3.227) and (3.228) from the Linard-Wiechert potential (10.138), we find the electromagnetic fields

$$\mathbf{E}(\mathbf{x},t) = \frac{e}{4\pi}\left[\frac{(\mathbf{n}-\bar{\mathbf{v}}/c)}{(1-\mathbf{n}\cdot\bar{\mathbf{v}}/c)^2}\frac{1}{R^2} + \frac{\mathbf{n}\times[(\mathbf{n}-\bar{\mathbf{v}}/c)\times\dot{\bar{\mathbf{v}}}]}{(1-\mathbf{n}\cdot\bar{\mathbf{v}}/c)^3}\frac{1}{R}\right]_{\rm ret} \tag{10.143}$$

$$\mathbf{B}(\mathbf{x},t) = \left[\frac{\mathbf{R}\times\mathbf{E}}{R}\right]_{\rm ret}, \tag{10.144}$$

The two terms in $\mathbf{E}(\mathbf{x},t)$ have different falloff behaviors in $1/R$ with increasing distance from the source. The first is a *velocity field* which falls off like $1/R^2$. It is essentially the moving static field around the particle. The second term is an *acceleration field*, which has a slower fall-off proportional to $1/R$. For this reason it can carry off radiation energy to infinity.

Indeed, the energy flux through a solid angle $d\Omega$ is given by the scalar product of the Poynting vector $\mathbf{E}\times\mathbf{B}$ with the area element $d\mathbf{S}$:

$$\dot{\mathcal{E}} = d\mathbf{S}\cdot(\mathbf{E}\times\mathbf{B}) = d\Omega\, c\,\mathbf{E}^2. \tag{10.145}$$

For a radiating electron at small velocities near the coordinate origin, the acceleration field simplifies to

$$\mathbf{E}(\mathbf{x},t) = \frac{e}{4\pi rc^2}[\hat{\mathbf{x}}\times(\hat{\mathbf{x}}\times\ddot{\mathbf{x}})], \quad \mathbf{B}(\mathbf{x},t) = \frac{e}{4\pi rc^2}(\hat{\mathbf{x}}\times\ddot{\mathbf{x}}). \tag{10.146}$$

with $r = |\mathbf{x}|$. The radiated power per solid angle is then

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{e^2}{(4\pi)^2 c^3}(\hat{\mathbf{x}} \times \ddot{\mathbf{x}})^2 = \frac{e^2}{(4\pi)^2 c^3}\,\ddot{\mathbf{x}}^2 \sin^2\beta, \tag{10.147}$$

where β is the angle between the oscillating dipole end the direction of emission. By integrating over all solid angles, we obtain the total radiated power

$$\dot{\mathcal{E}} = \frac{e^2}{(4\pi)^2 c^3}\int d\Omega\,(\hat{\mathbf{x}} \times \ddot{\mathbf{x}})^2 = \frac{2}{3c^3}\frac{e^2}{4\pi}\ddot{\mathbf{x}}^2. \tag{10.148}$$

This is the famous *Larmor formula* of classical electrodynamics.

For a harmonically oscillating charge at position

$$x(t) = x_0 e^{-i\omega t} + x_0^* e^{i\omega t} = 2|x_0|\cos(\omega t + \delta), \tag{10.149}$$

equation (10.147) yields the temporal average power

$$\frac{d\dot{\mathcal{E}}}{d\Omega} = \frac{e^2}{8\pi^2}\frac{\omega^4}{c^3}|\hat{\mathbf{x}} \times \mathbf{x}_0|^2 = \frac{e^2}{8\pi^2}\frac{\omega^4}{c^3}|\mathbf{x}_0|^2 \sin^2\beta, \tag{10.150}$$

and the total radiated power is

$$\dot{\mathcal{E}} = \frac{4}{3}\frac{e^2}{4\pi}\frac{\omega^4}{c^3}|\mathbf{x}_0|^2. \tag{10.151}$$

Note that with respect to many textbooks on classical electrodynamics where the electromagnetic Lagrangian carries a factor $1/4\pi$ on the right-hand side of (10.3), the square of the charge in the present standard normalization of quantum electrodynamics is related to the fine-structure constant α by $e^2 = 4\pi\alpha\hbar c$.

According to the correspondence principle, the same result hold for an atom decaying from level n to n', if we replace $|\mathbf{x}_0|$ by the absolute square of the quantum mechanical matrix element (10.133):

$$|\mathbf{x}_0|^2 \to \left|\sum_\nu \langle n'|\mathbf{x}^{(\nu)}|n\rangle\right|^2, \tag{10.152}$$

This yields the radiated power per unit solid angle

$$\frac{d\dot{\mathcal{E}}_{n'n}}{d\Omega} = \frac{e^2}{8\pi^2}\frac{\omega^4}{c^3}\left|\sum_\nu \langle n'|\mathbf{x}^{(\nu)}|n\rangle\right|^2 \sin^2\theta. \tag{10.153}$$

Let us now confirm this result by a proper calculation within quantum electrodynamics, We shall consider only a single electron in a hydrogen-like atom with central charge Ze. For a nonrelativistic electron of mass M moving in a Coulomb potential

$$V_{\rm C}(\mathbf{x}) \equiv -\frac{Z\alpha}{|\mathbf{x}|}, \tag{10.154}$$

the Hamiltonian reads in the transverse gauge with $\boldsymbol{\nabla}\mathbf{A}(x) = 0$,

$$H = \frac{\mathbf{p}^2}{2M} - \frac{1}{M}\mathbf{A}(\mathbf{x},t)\cdot\mathbf{p} + \frac{e^2}{2M}\mathbf{A}^2(\mathbf{x},t) + V_{\rm C}(\mathbf{x}) + A^0(\mathbf{x},t) = H_{\rm C} + H^{\rm int}. \quad (10.155)$$

where

$$H_{\rm C} = \frac{\mathbf{p}^2}{2M} + \mathbf{V}_{\rm C}(\mathbf{x}) \quad (10.156)$$

is the Hamiltonian of the hydrogen-like atom by itself, and $H^{\rm int}$ contains the interaction with the zeroth time-like component of the vector potential $A^0(\mathbf{x},t) = 0$, which is determined by the electronic charge distribution via the Coulomb law Eq. (10.69), and with the radiation field $\mathbf{A}(\mathbf{x},t) = 0$, which has an expansion in terms of photon creation and annihilation operators as in Eq. (5.336):

$$\mathbf{A}(\mathbf{x},t) = \sum_{\mathbf{k},h} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[e^{-ikx}\boldsymbol{\epsilon}(\mathbf{k},h)a_{\mathbf{k},h} + \text{h.c.}\right]. \quad (10.157)$$

Let $|n\rangle$. be an excited initial state of an atom with quantum number n, which decays into a lower state $a^\dagger(\mathbf{k},h)|n'\rangle$. with quantum number n' containing, in addition, a photon of wave vector $\mathbf{k}$, energy $\omega = ck$, and helicity h. According to Eq. (7.166), the decay probability of the initial state per unit time is given by Fermi's golden rule (in the remainder of this section we use physical units):

$$\frac{dP_{n'n}}{dt} = \int \frac{d^3kV}{(2\pi)^3} 2\pi\hbar\delta(E_n + \hbar\omega - E_{n'}) \left|\frac{1}{\hbar}\langle n'|a(\mathbf{k},h)R|n\rangle\right|^2, \quad (10.158)$$

where R is the $R-$matrix which coincides in lowest order perturbation theory with $H^{\rm int}$ [see (7.174)]. The matrix element is obviously

$$\langle n'|a(\mathbf{k},h)H^{\rm int}|n\rangle = \frac{c}{\sqrt{2V\omega}}\frac{e}{Mc}\langle n'|e^{-i\mathbf{kx}}\boldsymbol{\epsilon}^*(h)\cdot\mathbf{p}|n\rangle. \quad (10.159)$$

Performing the integral over the photon momentum (neglecting recoil) we find from (10.158) the differential decay rate [compare (7.239)]

$$\frac{d\Gamma_{n'n}}{d\Omega} = \frac{e^2}{8\pi^2\hbar}\frac{\omega}{M^2c^3}|\langle n'|e^{-i\mathbf{kx}}\boldsymbol{\epsilon}^*(h)\cdot\mathbf{p}|n\rangle|^2. \quad (10.160)$$

The further calculation is simplified by the observation that the wavelength of the emitted photons is the inverse of their energy (in massless units), and thus of the order of $\hbar/Z\alpha^2Mc$, about 100 times larger than the atomic diameter which is of the order of the Bohr radius $a_{\rm B} = \hbar/Z\alpha Mc$ for an atom of charge Z, The exponential $e^{-i\mathbf{kx}}$ is therefore almost unity and can dropped. This yields the *dipole approximation* to the atomic decay rate:

$$\frac{d\Gamma_{n'n}}{d\Omega} \approx \frac{e^2}{8\pi^2\hbar}\frac{\omega}{M^2c^3}|\boldsymbol{\epsilon}^*(h)\cdot\langle n'|\mathbf{p}|n\rangle|^2. \quad (10.161)$$

The momentum operator $\mathbf{p}$ can be replaced by $M\dot{\mathbf{x}} = i[H, \mathbf{x}]/\hbar$, and thus, in the matrix element $\langle n'|\mathbf{p}|n\rangle|^2$, by $iM(E_{n'} - E_n)\mathbf{x}/\hbar = -iM\omega\mathbf{x}$. Multiplying the decay rate by the energy of the photon $\hbar\omega$ to get the rate of radiated energy, the result (10.161) coincides with the classical result (10.153).

It is customary to introduce the so-called *oscillator strength* of a single component of the x-operator

$$f_{n'n} \equiv \frac{2M}{\hbar}\left|\sum_{\nu}\langle n'|x^{(\nu)}|n\rangle\right|^2 . \tag{10.162}$$

As a consequence of the canonical commutator $[p, x] = -i\hbar$, the oscillator strengths satisfy the *Thomas-Reiche-Kuhn sum rule*:

$$\sum_{n'} f_{n'n} = Z. \tag{10.163}$$

Let

$$\langle \mathbf{x}|nlm\rangle = R_{nl}(r)Y_{lm}(\theta, \varphi) \tag{10.164}$$

be the decomposition of the hydrogen wave functions into radial and angular parts. Then the matrix elements of $\mathbf{x}$ factorize:

$$\langle n'l'm'|\mathbf{x}|nlm\rangle = r_{n'l';nl} \times \langle l'm'|\hat{\mathbf{x}}|lm\rangle, \tag{10.165}$$

where the matrix elements of r,

$$r_{n'l';nl} \equiv \int drr^2 R_{n'l'}(r) r R_{nl}(r), \tag{10.166}$$

have been calculated by Gordon:[2]

$$\begin{aligned} r_{n'l';nl} &= \frac{(-1)^{n'-l}}{4(2l-1)!}\sqrt{\frac{(n+l)!(n'+l-1)!}{(n'-l)!(n-l-1)!}}(4nn')^{l+1}\frac{(n-n')^{n+n'-2l-2}}{(n+n')^{n+n'}} \\ &\times\left\{F\left(-n_r', 2l, -\frac{4nn'}{(n-n')^2}\right) - \left(\frac{n-n'}{n+n'}\right)^2 F\left(-n_r - 2, -n_r', 2l, -\frac{4nn'}{(n-n')^2}\right)\right\}, \end{aligned} \tag{10.167}$$

with $F(a, b, c; z)$ being hypergeometric functions. The angular matrix elements of the unit vector in (10.165),

$$\langle l'm'|\hat{\mathbf{x}}|lm\rangle \equiv \int d\hat{\mathbf{x}} Y^*_{l'm'}(\theta, \varphi)\hat{\mathbf{x}} Y_{lm}(\theta, \varphi). \tag{10.168}$$

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[2] W. Gordon, Ann. d. Phys. *2*, 1031 (1929). They can be found very simply by group theory, as shown by H. Kleinert, Fortschr. Phys. *6*, 1, (1968), and *Group Dynamics of the Hydrogen Atom*, Lectures presented at the 1967 Boulder Summer School, published in *Lectures in Theoretical Physics*, Vol. X B, pp. 427 482, ed. by A.O. Barut and W.E. Brittin, Gordon and Breach, New York, 1968.

are easily found, since $\hat{x}_3 = \cos\theta$ and the spherical harmonics satisfy the recursion relation

$$\cos\theta\, Y_{lm}(\theta,\varphi) = \sqrt{\frac{(l+1)^2-m^2}{(2l+2)(2l+1)}}Y_{l+1\,m}(\theta,\varphi) + \sqrt{\frac{l^2-m^2}{(2l+1)(2l-1)}}Y_{l-1\,m}(\theta,\varphi). \tag{10.169}$$

Using the orthonormality relation

$$\int d\hat{\mathbf{x}}\, Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi) = \delta_{l'l}\delta_{m'm}, \tag{10.170}$$

we obtain immediately the angular matrix elements of $\hat{x}_3$:

$$\begin{aligned}\langle l+1\ m|\hat{x}_3|lm\rangle &= \sqrt{\frac{(l+1)^2-m^2}{(2l+2)(2l+1)}},\\ \langle l-1\ m'|\hat{x}_3|lm\rangle &= \sqrt{\frac{l^2-m^2}{(2l+1)(2l-1)}},\end{aligned} \tag{10.171}$$

with all others vanishing. The matrix elements of $\hat{x}_1$ and $\hat{x}_2$ are found with the help of the commutation rule

$$[L_i, \hat{x}_j] = i\epsilon_{ijk}\hat{x}_k, \tag{10.172}$$

which states that $\hat{x}_i$ is a *vector operator*. As a consequence, the matrix elements satisfy the Wigner-Eckart theorem,

$$\langle l'm' \pm 1|\hat{x}^{m''}|lm\rangle = \langle l'm'|1m''; lm\rangle \hat{x}_{l'l}, \tag{10.173}$$

where $\langle l'm'|1m''; lm\rangle$ are Clebsch-Gordan coefficients (see Appendix 3C) and $\hat{x}^{m''}$ are the spherical components of $\hat{\mathbf{x}}$ [recall the definition in Eq. (3.828)]:

$$\hat{x}^3 = \cos\theta, \quad \hat{x}^{\pm} = \mp(x^2 \pm x^2)/\sqrt{2} = \sin\theta e^{\pm i\varphi}/\sqrt{2}. \tag{10.174}$$

Explicitly:

$$\begin{aligned}\langle l+1\ m\pm 1| \mp (x_1 \pm ix_2)|lm\rangle &= \sqrt{\frac{(l\pm m+2)(l\pm m+1)}{(2l+3)(2l+1)}},\\ \langle l-1\ m\pm 1| \mp (x_1 \pm ix_2)|lm\rangle &= \sqrt{\frac{(l\mp m)(l\mp m-1)}{(2l+1)(2l-1)}}.\end{aligned} \tag{10.175}$$

10.7 Rutherford Scattering

The scattering of electrons on the Coulomb potential of nuclei of charge Ze

$$V_{\rm C}(r) = -\frac{ZE^2}{4\pi r} = -\frac{Z\alpha}{r} \tag{10.176}$$

was the first atomic collision observed experimentally by Rutherford. The associated scattering cross section can easily be calculated in an estimated classical approximation.

10.7.1 Classical Cross Section

In a Coulomb potential the electronic orbits are hyperbola. If an incoming electron runs along the z-direction and is deflected by a scattering angle θ towards the x direction (see Fig. 10.5) the nucleus has the coordinates

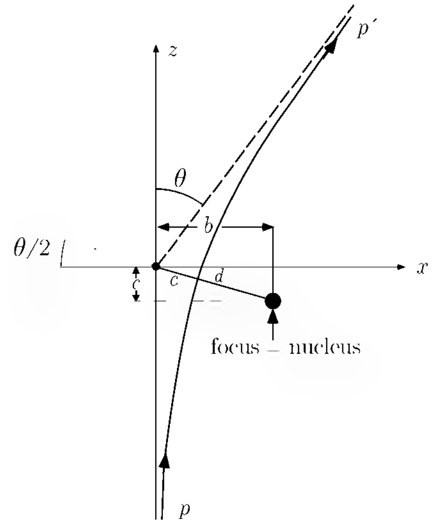


FIGURE 10.5 Kinematics of Rutherford cross section.

$$(x_{\rm F}, z_{\rm F}) = (b, -c) \tag{10.177}$$

where

$$\frac{c}{b} = \tan\frac{\theta}{2}, \qquad \frac{b}{d} = \cos\frac{\theta}{2}, \tag{10.178}$$

The distance of closest approach to the nucleus is

$$r_{\rm c} = d - c. \tag{10.179}$$

It is determined by the conservation of the nonrelativistic energy:

$$E^{\rm nr} = \frac{p^2}{2M} = \frac{p'^2}{2M} = \frac{p_{\rm c}^2}{2M} - \frac{Z\alpha}{r_{\rm c}}, \tag{10.180}$$

where p_c is the momentum at the point of closest approach. This momentum is determined by the conservation of the orbital angular momentum:

$$l = pb = p'b = p_c r_c. \tag{10.181}$$

From these equations we find

$$b = \frac{Z\alpha}{2E\tan(\theta/2)}. \tag{10.182}$$

The quantity b is called the *impact parameter* of the scattering process. It is the closest distance which an particle would have from the nucleus if it were not deflected at all. Particles which would pass through a thin annular ring with the radii b and $b + db$ are, in fact, scattered into a solid angle $d\Omega$ given by

$$db = -\frac{1}{4\pi}\frac{Z\alpha}{4E}\frac{1}{\sin^3(\theta/2)\cos(\theta/2)}d\Omega. \tag{10.183}$$

The current density of a single randomly incoming electron is $j = v/V$. It would pass through the annular ring, with a probability per unit time

$$d\dot{P} = j\,2\pi b db. \tag{10.184}$$

With this probability it winds up in the solid angle $d\Omega$. Inserting Eq. (10.183), we find the differential cross section [recall the definition Eq. (7.168)]

$$\frac{d\sigma}{d\Omega} = \frac{d\dot{P}}{d\Omega} = 2\pi b\frac{db}{d\Omega} = \frac{1}{4\sin^4(\theta/2)}\left(\frac{Z\alpha}{2E}\right)^2. \tag{10.185}$$

10.7.2 Quantum-Mechanical Born Approximation

Somewhat surprisingly, the same result is obtained in quantum mechanics within the Born approximation. According to Eqs. (7.170) and (7.175), the differential cross section is

$$\frac{d\sigma}{d\Omega} \approx \frac{M^2V^2}{(2\pi)^2}|V_{\mathbf{p}'\mathbf{p}}|^2, \tag{10.186}$$

where

$$V_{\mathbf{p}'\mathbf{p}} = -\frac{1}{V}\int d^3x\, e^{i(\mathbf{p}'-\mathbf{p})\mathbf{x}}\frac{Z\alpha}{r} = -\frac{4\pi}{V}\frac{Z\alpha}{|\mathbf{p}'-\mathbf{p}|^2}. \tag{10.187}$$

The quantity

$$|\mathbf{q}^2| \equiv |\mathbf{p}'-\mathbf{p}|^2 = 2p^2(1-\cos\theta) = 4p^2\sin^2(\theta/2) = 8EM\sin^2(\theta/2) \tag{10.188}$$

is the momentum transfer of the process. Inserting this into (10.187), the differential cross section (10.186) coincides indeed with the classical expression (10.185).

10.7.3 Relativistic Born Approximation

Let us now see how the above cross section formula is modified in a relativistic calculation involving Dirac electrons. The scattering amplitude is, according to Eq. (8.124),

$$S_{\rm fi} = -ie\langle \mathbf{p}', s_3'| \int d^4x\, \bar\psi(x)\gamma^\mu\psi(x)|\mathbf{p}, s_3\rangle A_\mu(x), \tag{10.189}$$

where $A_\mu(x)$ has only the time-like component

$$A^0(x) = -\frac{Ze}{4\pi r} = -\int \frac{d^3q}{(2\pi)^3}\, e^{i\mathbf{qx}} \frac{Ze}{|\mathbf{q}|^2}. \tag{10.190}$$

The time-ordering operator has been dropped in (10.189) since there are no operators at different times to be ordered in first-order perturbation theory. By evaluating the matrix element of the current and performing the spacetime integral we obtain

$$S_{\rm fi} = ie2\pi\delta(E'-E)\sqrt{\frac{M^2}{V^2E'E}}\bar u(\mathbf{p}', s_3')\gamma^0 u(\mathbf{p}, s_3)\frac{Ze}{|\mathbf{q}|^2}, \tag{10.191}$$

where E and E' are the initial and final energies of the electron, which are in fact equal in this elastic scattering process.

Comparing this with (7.111) we identify the R-matrix elements

$$R_{\mathbf{p}'\mathbf{p}} = \frac{M}{VE}\bar u(\mathbf{p}', s_3')\gamma^0 u(\mathbf{p}, s_3)\frac{Ze^2}{|\mathbf{q}|^2}, \tag{10.192}$$

This is to be compared with the nonrelativistic Barn approximation where (10.187) corresponds via (7.174) to

$$R_{\mathbf{p}'\mathbf{p}} = -\frac{1}{V}\frac{Ze^2}{|\mathbf{q}|^2}. \tag{10.193}$$

The relativistic amplitude receives therefore a correction factor

$$C = \frac{M}{E}\bar u(\mathbf{p}', s_3)\gamma^0 u(\mathbf{p}, s_3). \tag{10.194}$$

The absolute square of this multiplies the differential cross section. Apart from this, the relativistic cross section contains an extra kinematic factor E^2/M^2 accounting for the different phase space of a relativistic electron with respect to the nonrelativistic one [the ratio between (7.173) and (7.170)]. The differential cross section receives therefore a total relativistic correction factor

$$\frac{E^2}{M^2}C^2 = |\bar u(\mathbf{p}', s_3')\gamma^0 u(\mathbf{p}, s_3)|^2. \tag{10.195}$$

If we consider the scattering of unpolarized electrons and do not observe the final spin polarizations, this factor has to be summed over s_3' and averaged over s_3, and the correction factor is

$$\frac{E^2}{M^2}C^2 = \frac{1}{2}\sum_{s_3', s_3} \bar u(\mathbf{p}', s_3')\gamma^0 u(\mathbf{p}, s_3)\bar u(\mathbf{p}, s_3)\gamma^0 \bar u(\mathbf{p}', s_3'). \tag{10.196}$$

To write the absolute square in this form we have used the general identity in the spinor space, valid for any 4×4 spinor matrix M:

$$(\bar{u}' M u)^* = \bar{u} \bar{M} u', \tag{10.197}$$

where the operation "bar" is defined for a spinor matrix in complete analogy to the corresponding operation for a spinor:

$$\bar{M} \equiv \gamma^0 M^\dagger \gamma^{0-1}. \tag{10.198}$$

The Dirac matrices themselves satisfy

$$\bar{\gamma}^\mu = \gamma^\mu. \tag{10.199}$$

The bar operation has typical properties of "adjoining" operations. If it is applied to a product of matrices, the order is reversed:

$$\overline{M_1 \cdots M_n} = \overline{M}_n \cdots \overline{M}_1. \tag{10.200}$$

We use now the semi-completeness relation (3.641) for the u-spinors and rewrite (10.196) as

$$\frac{E^2}{M^2} C^2 = \frac{1}{2} \mathrm{tr} \left(\gamma^0 \frac{\not{p} + M}{2M} \gamma^0 \frac{\not{p} + M}{2M} \right). \tag{10.201}$$

The trace over product of gamma matrices occurring in this expression is typical for quantum electrodynamic calculations. Its evaluation is somewhat tedious, but follows a few quite simple algebraic rules.

The first states that a trace containing an odd number of gamma matrices vanishes. This is a simple consequence of the fact that γ^μ, and thus a product of any odd number of gamma matrices, changes sign under the similarity transformation $\gamma_5 \gamma^\mu \gamma_5 = -\gamma^\mu$, whereas the trace is invariant under any similarity transformation.

The second rule governs the evaluation of a trace containing an even number of gamma matrices. It is a recursive rule which makes essential use of the invariance of the trace under cyclic permutations

$$\mathrm{tr}\,(\gamma^{\mu_1} \gamma^{\mu_2} \gamma^{\mu_3} \cdots \gamma^{\mu_{n-1}} \gamma^{\mu_n}) = \mathrm{tr}\,(\gamma^{\mu_2} \gamma^{\mu_3} \cdots \gamma^{\mu_{n-1}} \gamma^{\mu_n} \gamma^{\mu_1}), \tag{10.202}$$

and leads to an explicit formula which is a close analog of Wick's expansion formula for a time ordered product of fermion field operators. For this purpose, we define a pair contraction between $\not{a}$ and $\not{b}$ as

$$\dot{\not{a}} \dot{\not{b}} \equiv \frac{1}{4} \mathrm{tr}\,(\not{a} \not{b}) = ab. \tag{10.203}$$

Then we may move the first gamma matrix in a trace such as

$$\frac{1}{4} \mathrm{tr}\,(\not{a}_1 \cdots \not{a}_n) \tag{10.204}$$

step by step to the end, using the anticommutation rules between gamma matrices (3.517), which imply

$$\not{a}_1\not{a}_i = -\not{a}_i\not{a}_1 + 2a_1a_i = -\not{a}_i\not{a}_1 + 2\dot{\not{a}}_1\dot{\not{a}}_i\,. \tag{10.205}$$

Having arrived at the end, it can be taken back to the front using the cyclic invariance of the trace. This produces once more the initial trace, except for a minus sign, thus doubling the initial trace on the left-hand side of the equation. In this way, we find the recursion relation

$$\begin{aligned}\frac{1}{4}\mathrm{tr}\,(\not{a}_1\not{a}_2\not{a}_3\cdots\not{a}_{n-1}\not{a}_n) &= \frac{1}{4}\mathrm{tr}\,(\dot{\not{a}}_1\dot{\not{a}}_2\not{a}_3\cdots\not{a}_{n-1}\not{a}_n) + \frac{1}{4}\mathrm{tr}\,(\dot{\not{a}}_1\not{a}_2\dot{\not{a}}_3\cdots\not{a}_{n-1}\not{a}_n)\\ &\dots + \frac{1}{4}\mathrm{tr}\,(\dot{\not{a}}_1\not{a}_2\not{a}_3\cdots\dot{\not{a}}_{n-1}\not{a}_n) + \dots + \frac{1}{4}\mathrm{tr}\,(\dot{\not{a}}_1\not{a}_2\not{a}_3\cdots\not{a}_{n-1}\dot{\not{a}}_n),\end{aligned} \tag{10.206}$$

whose explict form is

$$\begin{aligned}\frac{1}{4}\mathrm{tr}\,(\not{a}_1\not{a}_2\not{a}_3\cdots\not{a}_{n-1}\not{a}_n) &= (a_1a_2)\frac{1}{4}\mathrm{tr}\,(\not{a}_3\not{a}_4\cdots\not{a}_{n-1}\not{a}_n) + (a_1a_3)\frac{1}{4}\mathrm{tr}\,(\not{a}_2\not{a}_4\cdots\not{a}_{n-1}\not{a}_n)\\ &\dots + (a_1a_{n-1})\frac{1}{4}\mathrm{tr}\,(\not{a}_2\not{a}_3\cdots\not{a}_{n-2}\not{a}_n) + (a_1a_n)\frac{1}{4}\mathrm{tr}\,(\not{a}_2\not{a}_3\cdots\not{a}_{n-1}\not{a}_n).\end{aligned} \tag{10.207}$$

The contractions within the traces are defined as in (10.203), but with a minus sign for each permutation necessary to bring the Dirac matrices to adjacent positions. By repeating this process, we arrive at the expansion rule

$$\frac{1}{4}\mathrm{tr}\,(\not{a}_1\cdots\not{a}_n) = \sum_{\text{pair contractions}} (-)^P\,(a_{p(1)}a_{p(2)})(a_{p(3)}a_{p(4)})\cdots(a_{p(n-1)}a_{p(n)}). \tag{10.208}$$

where P is the number of permutations to adjacent positions.

The derivation of the rule is completely parallel to that of the thermodynamic version of Wick's rule in Section 4.14, whose Eqs. (5.778) and (5.779) can directly be translated into anticommutation rules between gamma matrices and the cyclic invariance of their traces, respectively.

Another set of useful rules following from (10.205) which will be needed later is

$$\begin{aligned}\gamma^\mu\not{a}\gamma^\nu &= \not{a} + 2a^\mu\gamma^\nu, &(10.209)\\ \gamma^\mu\gamma_\mu &= 4, &(10.210)\\ \gamma^\mu\not{a}\gamma_\mu &= -2\not{a}\,, &(10.211)\\ \gamma^\mu\not{a}\not{b}\gamma_\mu &= -2\not{a}\,, &(10.212)\\ \gamma^\mu\not{a}\not{b}\not{b}\gamma_\mu &= -2\not{c}\not{b}\not{a}\,. &(10.213)\end{aligned}$$

With the Wick rule (10.244) for γ-matrices we now calculate the expression (10.201) as f

$$\begin{aligned}\frac{E^2}{M^2}C^2 &= \frac{1}{2M^2}\left[\frac{1}{4}\mathrm{tr}\,(\gamma^0\not{p}\gamma^0\not{p}') + M^2\mathrm{tr}\,(\gamma^{02})\right]\\ &= \frac{1}{2M^2}\left(2p^0p'^0 - pp' + M^2\right).\end{aligned} \tag{10.214}$$

Inserting $p^0 = p'^0 = E$ and, in the center-of-mass frame,

$$pp' = E^2 - |\mathbf{p}|^2 \cos\theta = M^2 + 2|\mathbf{p}|^2 \sin^2\frac{\theta}{2}, \tag{10.215}$$

and the total cross section in the center-of-mass frame

$$\frac{d\sigma}{d\Omega_{\rm CM}} = \frac{Z^2\alpha^2 M^2}{4|\mathbf{p}|^4 \sin^4(\theta/2)} \times \frac{E^2}{M^2} C^2. \tag{10.216}$$

This relativistic version of Rutherford's formula is known as *Mott's formula.*

In terms of the incident electron velocity, the total modification factor reads

$$\frac{E^2}{M^2} C^2 = \frac{1}{1-(v/c)^2} \left[1 - \left(\frac{v}{c}\right)^2 \sin^2\frac{\theta}{2}\right]. \tag{10.217}$$

It is easy to verify that the same differential cross section is valid for positrons. In the nonrelativistic case, this follows directly from the invariance of (10.186) under $e \to -e$. But also the relativistic correction factor remains the same under the interchange of electrons and positrons, where (10.196) becomes

$$\frac{E^2}{M^2} C^2 = \frac{1}{2} \sum_{s_3', s_3} \bar{v}(\mathbf{p}', s_3')\gamma^0 v(\mathbf{p}, s_3)\bar{v}(\mathbf{p}, s_3)\gamma^0 \bar{v}(\mathbf{p}', s_3'). \tag{10.218}$$

Inserting the semi-completeness relation (3.642) for the spinors $v(\mathbf{p}, s_3)$, this becomes

$$\frac{E^2}{M^2} C^2 = \frac{1}{2} \mathrm{tr} \left(\gamma^0 \frac{\not{p} - M}{2M} \gamma^0 \frac{\not{p}' - M}{2M}\right), \tag{10.219}$$

which is the same as (10.196) since only traces of an even number of gamma matrices contribute.

10.8 Compton Scattering

A simple scattering process whose cross section can be calculated to a good accuracy by means of the above diagrammatic rules is photon-electron scattering, also referred to as *Compton scattering*. It gives an important contribution to the blue color of the sky.

Consider now a beam of photons with four-momentum $k_{\rm i}$ and polarization $\lambda_{\rm i}$ impinging upon an electron target of four-momentum $p_{\rm i}$ and spin orientation $\sigma_{\rm i}$. The two particles leave the scattering regime with four-momenta $k_{\rm f}, p_{\rm f}$, and spin indices $\lambda_{\rm f}, \sigma_{\rm f}$, respectively. Adapting formula (8.91) for the scattering amplitude to this situation we have

$$\begin{aligned} S_{\rm fi} &= S\left(\mathbf{p}', s_3'; \mathbf{k}', h' | \mathbf{k}, h; \mathbf{p}, s_3\right) \\ &\equiv \frac{\langle 0 | a(\mathbf{p}', s_3') a(\mathbf{k}', h') \hat{T} e^{-i\int_{-\infty}^{\infty} dt V_I(t)} a^\dagger(\mathbf{k}, h) a^\dagger(\mathbf{p}, s_3) | 0\rangle}{\langle 0 | e^{-i\int_{-\infty}^{\infty} dt V_I(t)} | 0\rangle} \\ &\equiv S_N\left(\mathbf{p}', s_3'; \mathbf{k}', h' | \mathbf{k}, h; \mathbf{p}, s_3\right) / Z[0]. \end{aligned} \tag{10.220}$$

with

$$e^{-i\int_{-\infty}^{\infty}dt\,V_I(t)}=e^{-ie\int d^4x\,\bar{\psi}(x)\gamma^\mu\psi(x)A^\mu(x)}. \tag{10.221}$$

Expanding the exponential in powers of e, we see that the lowest-order contribution to the scattering amplitude comes from the second-order term which gives rise to the two Feynman diagrams shown in Fig. (10.6). In the first, the electron s_1 of momentum p absorbs a photon of momentum k, and emits a second photon of momentum k', to arrive in the final state of momentum p'. In the second diagram, the acts of emission and absorption have the reversed order. Before we calculate the scattering cross section associated with these Feynman diagrams, let us first recall the classical result.

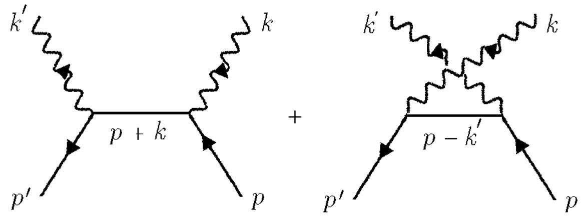


FIGURE 10.6 Lowest-order Feynman Diagrams contributing to Compton Scattering and giving rise to the Klein-Nishina formula.

10.8.1 Classical Result

Classically, the above process is described as follows. A target electron is shaken by an incoming electromagnetic field. The acceleration of the electron causes an emission of antenna radiation. For a weak and slowly oscillating electromagnetic field of amplitude, the electron is shaken nonrelativistically and moves with an instantaneous acceleration

$$\ddot{\mathbf{x}}=\frac{e}{M}\mathbf{E}=\frac{e}{M}\boldsymbol{\epsilon}\,E_0e^{-i\omega t+i\mathbf{k}\cdot\mathbf{x}}, \tag{10.222}$$

where ω is the frequency and E_0 the amplitude of the incoming field.

The acceleration of the charge gives rise to antenna radiation following Larmor's formula. Inserting (10.222) into (10.145), and averaging over the temporal oscillations, the radiated power per unit solid angle is

$$\frac{d\dot{\mathcal{E}}}{d\Omega}=\frac{1}{2}\left(\frac{e^2}{4\pi M}\right)^2E_0^2\sin^2\beta, \tag{10.223}$$

where β is the angle between the direction of polarization of the incident light and the direction of the emitted light.

For a later comparison with quantum electrodynamic calculations we associate this emitted power with a differential cross section of the electron. According to the definition in Chapter 6, a cross section is obtained by dividing the radiated power per unit solid angle by the incident power flux density. This yields

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi M}\right)^2 \sin^2\beta = r_e^2 \sin^2\beta, \tag{10.224}$$

where

$$r_e = \frac{e^2}{4\pi Mc^2} = \frac{\hbar\alpha}{Mc} \approx 2.82 \times 10^{-13}\ \mathrm{cm} \tag{10.225}$$

is the *classical electron radius*. Formula (10.224) describes the so-called *Thomson scattering cross section*.

Formula (10.224) holds for incident light which is linearly polarized. For unpolarized light, we have take the average between the cross section (10.224) and another one in which the plane of polarization is rotated by 90%. Suppose the incident light runs along the z-axis, and the emitted light along the direction $\hat{\mathbf{k}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. For a polarization direction $\boldsymbol{\epsilon} = \hat{\hat{\mathbf{x}}}$ along the x-axis, the angle β is found from

$$\sin^2\beta = (\hat{\mathbf{k}} \times \boldsymbol{\epsilon})^2 = \cos^2\theta + \sin^2\theta\sin^2\phi. \tag{10.226}$$

For a polarization direction $\boldsymbol{\epsilon} = \hat{\hat{\mathbf{x}}}$ along the y-axis, it is

$$\sin^2\beta = (\hat{\mathbf{k}} \times \boldsymbol{\epsilon})^2 = \cos^2\theta + \sin^2\theta\cos^2\phi. \tag{10.227}$$

The average is

$$\overline{\sin^2\beta} = \cos^2\theta + \frac{1}{2}\sin^2\theta = \frac{1}{2}(1+\cos^2\theta). \tag{10.228}$$

Integrating this over all solid angles yields the Thomson cross section for unpolarized light

$$\sigma_{\rm tot} = \frac{8\pi}{3} r_e^2. \tag{10.229}$$

10.8.2 Klein-Nishina Formula

The scattering amplitude corresponding to the two Feynman diagrams in Fig. 10.6) is obtained by expanding formula (8.91) up to second order in e:

$$S_{\rm fi} = -e^2 \int d^4x d^4y \langle 0|a_{\mathbf{p}',s_3'} \hat{T} \bar\psi(y) \not{\epsilon}' \psi(y) \bar\psi(x) \not{\epsilon}\, \psi(x) a^\dagger_{\mathbf{p},s_3}|0\rangle, \tag{10.230}$$

and performing the Wick contractions of Section 7.8:

$$\begin{aligned} &\langle 0|a_{\mathbf{p}',s_3'} \hat{T} \bar\psi(y) \not{\epsilon}' \psi(y) \bar\psi(x) \not{\epsilon}\, \psi(x) a^\dagger_{\mathbf{p},s_3}|0\rangle \qquad (10.231)\\ &= \langle 0|\hat{T} \dot{a}_{\mathbf{p}',s_3'} \dot{\bar\psi}(y) \not{\epsilon}' \overset{\therefore}{\psi}(y) \overset{\therefore}{\bar\psi}(x) \not{\epsilon}\, \ddot{\psi}(x) \ddot{a}^\dagger_{\mathbf{p},s_3}|0\rangle + \langle 0|\hat{T} \dot{a}_{\mathbf{p}',s_3'} \overset{\therefore}{\bar\psi}(y) \not{\epsilon}' \ddot{\psi}(y) \dot{\bar\psi}(x) \not{\epsilon}\, \overset{\therefore}{\psi}(x) \ddot{a}^\dagger_{\mathbf{p},s_3}|0\rangle. \end{aligned}$$

After Fourier expanding the intermediate electron propagator,

$$G_0(y,x) = \int \frac{d^4p^{\rm i}}{(2\pi)^4} e^{-ip^{\rm i}(y-x)} \frac{i}{\not{p}^{\rm i} - M}, \tag{10.232}$$

we find

$$
\begin{aligned}
S_{\rm fi} &= -e^2 \int d^4x d^4y e^{k'y-kx} \int \frac{d^4p^{\rm i}}{(2\pi)^4} \frac{M}{\sqrt{V^2EE'2\omega 2\omega'}} \\
&\times \left[e^{i(p'-p^{\rm i})y-(p-p^{\rm i})x} \bar{u}(\mathbf{p}', s_3') \not{\epsilon}'^* \frac{i}{\not{p}^{\rm i} - M} \not{\epsilon} u(\mathbf{p}, s_3) \right. \\
&\left. + e^{i(p'-p^{\rm i})x-(p-p^{\rm i})y} \bar{u}(\mathbf{p}', s_3') \not{\epsilon} \frac{i}{\not{p}^{\rm i} - M} \not{\epsilon}' u(\mathbf{p}, s_3) \right]. \qquad (10.233)
\end{aligned}
$$

One of the spatial integrals fixes the intermediate momentum in accordance with energy-momentum conservation, the other yields a $\delta^{(4)}$-function for overall energy-momentum conservation. The result is

$$
S_{\rm fi} = -i(2\pi)^4 \delta^{(4)}(p' + k' - p - k) e^2 \frac{M}{\sqrt{V^2 EE'2\omega 2\omega'}} \bar{u}(\mathbf{p}', s_3') H u(\mathbf{p}, s_3), \qquad (10.234)
$$

where H is the 4×4-matrix in spinor space

$$
H \equiv \not{\epsilon}'^* \frac{(\not{p} + \not{k}) + M}{(p + k)^2 - M^2} \not{\epsilon} + \not{\epsilon} \frac{(\not{p} - \not{k}') + M}{(p - k')^2 - M^2} \not{\epsilon}'^*. \qquad (10.235)
$$

We have written $\epsilon(\mathbf{k}, h)$, $\omega_{\mathbf{k}}$ as ϵ, ω, and $\epsilon(\mathbf{k}', h')$, $\omega_{\mathbf{k}'}$ as ϵ', ω', respectively, with a similar simplification for E and E'. The second term of the matrix H arises from the first by the *crossing symmetry*

$$
\epsilon \leftrightarrow \epsilon', \qquad k \leftrightarrow -k'. \qquad (10.236)
$$

Simplifications arise from the properties (10.237) It can, moreover, be simplified by recalling that external electrons and photons are on their mass shell, so that

$$
p^2 = p'^2 = M^2, \quad k^2 = k'^2 = 0, \qquad (10.237)
$$

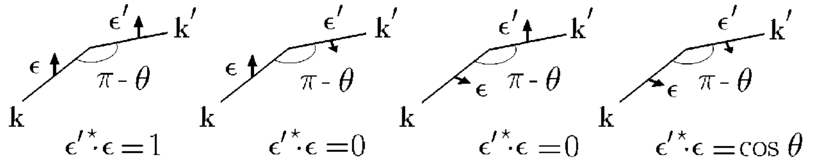
$$
k\epsilon = k'\epsilon' = 0. \qquad (10.238)
$$

A further simplification arises by working in the laboratory frame in which the initial electron is at rest, $p = (M, 0, 0, 0)$. Also, we choose a gauge in which the polarization vectors have only spatial components. Then

$$
p\epsilon = p\epsilon' = 0, \qquad (10.239)
$$

since p has only a temporal component and ϵ only space components. We also use the fact that H stands between spinors which satisfy the Dirac equation $(\not{p} - M)u(\mathbf{p}, s_3) = 0$, $\bar{u}(\mathbf{p}, s_3)(\not{p} - M) = 0$. Further we use the commutation rules (3.517) for the gamma matrices to write, as in (10.205),

$$
\not{p}\not{\epsilon} = -\not{\epsilon}\not{p} + 2p\epsilon. \qquad (10.240)
$$



ϵ'
k'
ϵ
$\pi-\theta$
k
$\epsilon'^{*}\cdot\epsilon=1$
$\epsilon'^{*}\cdot\epsilon=0$
$\epsilon'^{*}\cdot\epsilon=0$
$\epsilon'^{*}\cdot\epsilon=\cos\theta$

FIGURE 10.7 Illustration of the photon polarization sum $\sum_{h,h'}|\boldsymbol{\epsilon}'^{*}\boldsymbol{\epsilon}|^2 = 1+\cos^2\theta$ in Compton scattering in the laboratory frame. Incoming and outgoing photon momenta with scattering angle θ are shown in the scattering plane, together with their transverse polarization vectors.

The second term vanishes by virtue of Eq. (10.239). Similarly, we see that $\not{p}'$ anticommutes with $\not{\epsilon}'$. Using these results, we may eliminate the terms $\not{p}+M$ occurring in M. Finally, using Eq. (10.238), we obtain

$$\bar{u}(\mathbf{p}',s_3')Hu(\mathbf{p},s_3) \;=\; \bar{u}(\mathbf{p}',s_3')\left\{\not{\epsilon}'^{*}\frac{\not{k}}{2pk}\not{\epsilon}+\not{\epsilon}\frac{\not{k}'}{2pk'}\not{\epsilon}'^{*}\right\}u(\mathbf{p},s_3). \qquad (10.241)$$

To obtain the transition probability, we must take the absolute square of this. If we do not observe initial and final spins, we may average over the initial and sum over the final spin components which produces a factor 1/2 times the double sum: so that we and form

$$F=\sum_{s_3',s_3}|\bar{u}(\mathbf{p}',s_3')Hu(\mathbf{p},s_3)|^2=\sum_{s_3',s_3}\bar{u}(\mathbf{p}',s_3')Hu(\mathbf{p},s_3)\bar{u}(\mathbf{p},s_3)Hu(\mathbf{p}',s_3'). \qquad (10.242)$$

Now we use the semi-completeness relation (3.641) for the spinors to rewrite (10.242) as

$$F \;=\; \frac{1}{4M^2}\mathrm{tr}\left[(\not{p}'+M)H(\not{p}+M)H\right]. \qquad (10.243)$$

The trace over product of gamma matrices can be evaluated according to the Wick-type of rules explained on p. 585.

$$\frac{1}{4}\mathrm{tr}\,(\not{a}_1\cdots\not{a}_n)=\sum_{\text{pair contractions}}(-)^P\not{a}_1\cdots\not{a}_n. \qquad (10.244)$$

After some lengthy algebra (see Appendix 9A), we find

$$F=\frac{1}{2M^2}\left[\frac{\omega'}{\omega}+\frac{\omega}{\omega'}-2+4|\boldsymbol{\epsilon}'^{*}\cdot\boldsymbol{\epsilon}|^2\right], \qquad (10.245)$$

This holds for specific polarizations of the incoming and outgoing photons. If we sum over all final polarizations and average over all initial ones, we find (see Fig. 10.7)

$$\frac{1}{2}\sum_{h,h'}|\boldsymbol{\epsilon}'^{*}\boldsymbol{\epsilon}|^2=\frac{1}{2}(1+\cos^2\theta), \qquad (10.246)$$

This can also be found more formally using the transverse completeness relation (??) of the polariztion vectors:

$$\frac{1}{2}\sum_{h,h'}|\boldsymbol{\epsilon}'^*\boldsymbol{\epsilon}|^2=\frac{1}{2}\sum_{h,h'}\epsilon'^{i*}(\mathbf{k}',h')\epsilon^i(\mathbf{k},h)\epsilon^{*j}(\mathbf{k},h)\epsilon'^i(\mathbf{k}',h')=\frac{1}{2}\left(\delta^{ij}-\frac{k^ik^j}{\mathbf{k}^2}\right)\left(\delta^{ji}-\frac{k'^jk'^i}{\mathbf{k}'^2}\right)$$
$$=\frac{1}{2}\left[1+\frac{(\mathbf{k}\cdot\mathbf{k}')^2}{\mathbf{k}^2\mathbf{k}'^2}\right]=\frac{1}{2}(1+\cos^2\theta), \tag{10.247}$$

The average value of F is therefore

$$\bar{F}=\frac{1}{2}\sum_{h,h'}\frac{1}{2M^2}\left[\frac{\omega'}{\omega}+\frac{\omega}{\omega'}-2+4|\boldsymbol{\epsilon}'^*\cdot\boldsymbol{\epsilon}|^2\right]=\frac{1}{M^2}\left[\frac{\omega'}{\omega}+\frac{\omega}{\omega'}-\sin^2\theta\right]. \tag{10.248}$$

We are now ready to calculate the transition rate, for which we obtain from Eq. (7.201)

$$\frac{dP}{dt}=V(2\pi)^4\int\frac{d^3p'V}{(2\pi)^3}\int\frac{d^3k'V}{(2\pi)^3}\delta^{(4)}(p'-p)|t_{\rm fi}|^2, \tag{10.249}$$

with the squared t-matrix elements

$$|t_{\rm fi}|^2=e^4\frac{1}{V^4}\frac{M^2}{EE'2\omega 2\omega'}\frac{1}{2}F. \tag{10.250}$$

The spatial part of the δ-function removes the momentum integral over $\mathbf{p}'$. The temporal part of the δ-function enforces energy conservation. This is incorporated into the momentum integral over $\mathbf{k}'$ as follows. We set $E_{\rm f}=p'_0+k'_0$, and write

$$d^3k'=k'^2dk'd\Omega=\omega'^2\frac{d\omega'}{dE_{\rm f}}d\Omega dE_{\rm f}, \tag{10.251}$$

where Ω is the solid angle into which the photon has been scattered. Then (10.249) becomes

$$\frac{dP}{dtd\Omega}=Ve^4(2\pi)^4\frac{V^2}{(2\pi)^6}\left(\frac{\omega'}{\omega}\right)\left.\frac{d\omega'}{dE_{\rm f}}\right|_{E_{\rm f}=E_{\rm i}}\frac{1}{4V^4}\frac{M^2}{EE'}\frac{1}{2}F. \tag{10.252}$$

For an explicit derivative $d\omega'/dE_{\rm f}$, we go to the laboratory frame and express the final energy as

$$E_{\rm f}=\omega'+\sqrt{\mathbf{p}'^2+M^2}=\omega'+\sqrt{(\mathbf{k}-\mathbf{p}')^2+M^2}=\omega'+\sqrt{\omega^2-2\omega\omega'\cos\theta+\omega'^2+M^2}, \tag{10.253}$$

where θ is the scattering angle in the laboratory. Hence:

$$\frac{dE_{\rm f}}{d\omega'}=1+\frac{\omega'-\omega\cos\theta}{E'} \tag{10.254}$$

By equating $E_\mathrm{i} = M + \omega$ with E_f, we derive the *Compton relation*

$$\omega\omega'(1-\cos\theta) = M(\omega-\omega'), \tag{10.255}$$

or

$$\omega' = \frac{\omega}{1+\omega(1-\cos\theta)/M}, \tag{10.256}$$

and therefore

$$\frac{dE_\mathrm{f}}{d\omega'} = 1 + \frac{\omega' - \omega\cos\theta}{E'} = \frac{E' + \omega' - \omega\cos\theta}{E'} = \frac{M+\omega-\omega\cos\theta}{E'} = \frac{M}{E'}\frac{\omega}{\omega'}. \tag{10.257}$$

Since $E = M$ in the laboratory frame, Eq. (10.252) yields the differential probability rate

$$\frac{dP}{dtd\Omega} = Ve^4(2\pi)^4\frac{V^2}{(2\pi)^6}V\left(\frac{\omega'}{\omega}\right)^2\frac{1}{4V^4}\frac{1}{2}F. \tag{10.258}$$

To find the differential cross section, this has to be divided by the incoming particle current density. According to Eq. (7.218), this is given by

$$j = \frac{v}{V}, \tag{10.259}$$

where v is the velocity of the incoming particles. The incoming photons move with light velocity, so that (in natural units with $c = 1$)

$$j = \frac{1}{V}. \tag{10.260}$$

This leaves us with the *Klein-Nishina formula* for the differential cross section

$$\frac{d\sigma}{d\Omega} = \alpha^2\left(\frac{\omega'}{\omega}\right)^2\frac{1}{2}F. \tag{10.261}$$

In the nonrelativistic limit where $\omega << M$, the Compton relation (10.256) shows that $\omega' \approx \omega$, and Eq. (10.248) reduces to

$$F \longrightarrow \frac{1}{M^2}(1+\cos^2\theta). \tag{10.262}$$

Expressed in terms of the classical electron radius $r_0 = \alpha/M$, the differential scattering cross section becomes, expressed in terms of the classical electron radius where $r_0 = \alpha/M$,

$$\frac{d\sigma}{d\Omega} \approx {r_0}^2\,\frac{1}{2}(1+\cos^2\theta), \tag{10.263}$$

which is the Thomson formula for the scattering of low energy radiation by a static charge. To find the total Thomson cross section, we must integrate (10.263) over all solid angles:

$$\sigma = \int d\Omega\frac{d\sigma}{d\Omega} \approx 2\pi\int_{-1}^{1} d\cos\theta\; r_0^2\,\frac{1}{2}(1+\cos^2\theta), \tag{10.264}$$

which yields

$$\sigma_{\rm Thomson} \approx {r_0}^2 \frac{8\pi}{3}. \tag{10.265}$$

Let us also calculate the total cross section for relativistic scattering, integrating (10.261) over all solid angles:

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 2\pi \int_{-1}^{1} d\cos\theta \, \alpha^2 \frac{1}{2M^2} \left[\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - \sin^2\theta \right]. \tag{10.266}$$

Inserting

$$\omega' = \frac{\omega}{1 + \omega(1-\cos\theta)/M}, \tag{10.267}$$

which follows from (10.256), the angular integral yields

$$\sigma = \sigma_{\rm Thomson} f(\omega), \tag{10.268}$$

where $f(\omega)$ contains the relativistic corrections to Thomson's cross section:

$$f(\omega) = \left\{ \frac{1+\omega}{\omega^3} \left[\frac{2\omega(1+\omega)}{1+2\omega} - \log(1+2\omega) \right] + \frac{\log(1+2\omega)}{2\omega} - \frac{1+3\omega}{(1+2\omega)^2} \right\}. \tag{10.269}$$

For small ω:

$$f(\omega) = 1 - 2\omega + \mathcal{O}(\omega^2). \tag{10.270}$$

For large ω, $f(\omega)$ decreases like

$$f(\omega) = \frac{3}{8\omega} \left[\log 2\omega + \mathcal{O}(\log \omega/\omega) \right]. \tag{10.271}$$

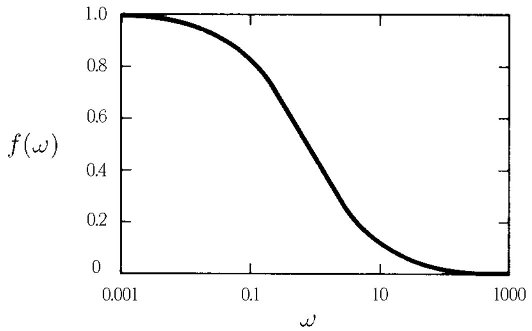


FIGURE 10.8 Ratio between total relativistic Compton cross section and nonrelativistic Thomson cross section.

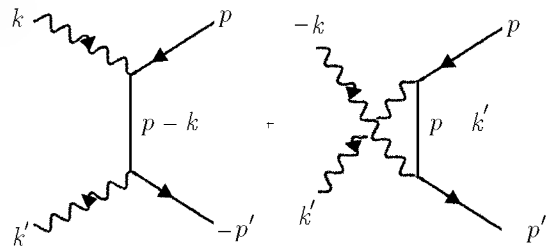


FIGURE 10.9 Lowest-Order Feynman Diagrams contributing to Electron-Positron Annihilation. It arises from the Compton diagram by the crossing operation $p' \to -p'$, $k \to -k$, $\epsilon \to \epsilon^*$.

10.9 Electron-Positron Annihilation

The Feynman diagram in Fig. 10.6 can also be read from bottom to top in which case it describes the annihilation of process corresponding to the two Feynman diagrams in Fig. 10.6). In order use as much as possible the previous results, we redraw the Feynman diagrams as shown in Fig. 10.9. Instead of an outgoing electron with momentum p' we let a negative-energy electron go out with momentum $-p'$. Instead of an incoming photon with momentum k we let a negative-energy photon go out with momentum $-k$. The former are represented by spinors $\bar{v}(\mathbf{p}', s_3)$, which are negative energy solutions of the Dirac equation with inverted momenta and spin directions. The S-matrix element to lowest order is from a slightly modified (10.230) as

$$S_{\rm fi} = -e^2 \int d^4x d^4y \langle 0|\hat{T}\bar{\psi}(y)\not{\epsilon}'\psi(y)\bar{\psi}(x)\not{\epsilon}\,\psi(x)b^\dagger_{\mathbf{p}',s_3'}a_{\mathbf{p},s_3}|0\rangle, \tag{10.272}$$

and performing the Wick contractions as in (10.232) we obtain

$$\begin{aligned} S_{\rm fi} \;=\; & -e^2 \int d^4x d^4y e^{k'y+kx} \int \frac{d^4p^{\rm i}}{(2\pi)^4} \frac{M}{\sqrt{V^2EE'2\omega 2\omega'}} \\ & \times \left[e^{i(-p'-p^{\rm i})y-(p-p^{\rm i})x} \bar{v}(\mathbf{p}', s_3')\not{\epsilon}'^* \frac{i}{\not{p}^{\rm i} - M} \not{\epsilon}^* u(\mathbf{p}, s_3) \right. \\ & \left. + e^{i(-p'-p^{\rm i})x-(p-p^{\rm i})y} \bar{v}(\mathbf{p}', s_3')\not{\epsilon}^* \frac{i}{\not{p}^{\rm i} - M} \not{\epsilon}' u(\mathbf{p}, s_3) \right]. \end{aligned} \tag{10.273}$$

Note that this arises from the Compton expression (10.233) by the crossing operation

$$p' \to -p', \;\; \bar{u}(\mathbf{p}, s_3) \to \bar{v}(\mathbf{p}, s_3), \qquad k \to -k, \;\; \epsilon(k,h) \to \epsilon^*(k,h). \tag{10.274}$$

As before, one of the spatial integrals fixes the intermediate momentum in accordance with energy-momentum conservation, the other yields a $\delta^{(4)}$-function for overall energy-momentum conservation. The result is

$$S_{\rm fi} = -i(2\pi)^4\delta^{(4)}(k+k'-p-p')e^2 \frac{M}{\sqrt{V^2EE'2\omega 2\omega'}} \bar{v}(\mathbf{p}', s_3')Hu(\mathbf{p}, s_3), \tag{10.275}$$

where H is the 4×4-matrix in spinor space

$$H \equiv \not{\epsilon}'^{*}\frac{(\not{p}-\not{k})+M}{(p-k)^2-M^2}\not{\epsilon}^{*}+\not{\epsilon}^{*}\frac{(\not{p}-\not{k}')+M}{(p-k')^2-M^2}\not{\epsilon}'^{*}. \tag{10.276}$$

As before, we have written $\epsilon(\mathbf{k},h)$, $\omega_{\mathbf{k}}$ as ϵ,ω, and $\epsilon(\mathbf{k}',h')$, $\omega_{\mathbf{k}'}$ as ϵ',ω', respectively, with a similar simplification for E and E'. The second term of the matrix H arises from the first by the *Bose symmetry*

$$\epsilon \leftrightarrow \epsilon', \qquad k \leftrightarrow k'. \tag{10.277}$$

Simplifications arise from the mass shell properties (10.237), the gauge conditions (10.238), and the other relations (10.239), (10.240). We also work again in the laboratory frame in which the initial electron is at rest, $p=(M,0,0,0)$ and the positron comes in with momentum $\mathbf{p}'$ and energy $E'=\sqrt{\mathbf{p}'^2+M^2}$. This leads to

$$\bar{v}(\mathbf{p}',s_3')Hu(\mathbf{p},s_3) \;=\; \bar{v}(\mathbf{p}',s_3')\left\{\epsilon'^{*}\frac{\not{k}}{2pk}\not{\epsilon}^{*}+\not{\epsilon}^{*}\frac{\not{k}'}{2pk'}\not{\epsilon}'^{*}\right\}u(\mathbf{p},s_3). \tag{10.278}$$

To obtain the transition probability, we must take the absolute square of this. If we do not observe initial spins, we may average over the initial spin components which gives a factor 1/4 times the spin sum

$$F=\sum_{s_3',s_3}|\bar{v}(\mathbf{p}',s_3')Hu(\mathbf{p},s_3)|^2=\sum_{s_3',s_3}\bar{v}(\mathbf{p}',s_3')Hu(\mathbf{p},s_3)\bar{u}(\mathbf{p},s_3)Hu(\mathbf{p}',s_3'). \tag{10.279}$$

Now we use the semi-completeness relations (3.641) and (3.642) for the spinors to rewrite (10.279) as

$$F \;=\; -\frac{1}{4M^2}\operatorname{tr}\left[(-\not{p}'+M)H(\not{p}+M)H\right]. \tag{10.280}$$

The trace over product of gamma matrices is now evaluated as before and we obtain for specific polarizations of the two outgoing photons. almost the same expression as before in Eq. (10.248) (see Appendix 9A):

$$F=\frac{1}{2M^2}\left[\frac{\omega'}{\omega}+\frac{\omega}{\omega'}+2-4|\boldsymbol{\epsilon}'^{*}\cdot\boldsymbol{\epsilon}^{*}|^2\right], \tag{10.281}$$

This result can be deduced directly from the previous polarization sum (10.245) by the crossing operation (10.274), apart from an overall minus sign, whose origin is the negative sign in front of (10.280).

We are now ready to calculate the transition rate, for which we obtain from Eq. (7.201)

$$\frac{dP}{dt}=V(2\pi)^4\int\frac{d^3k'V}{(2\pi)^3}\int\frac{d^3k'V}{(2\pi)^3}\delta^{(4)}(p'-p)|t_{\rm fi}|^2, \tag{10.282}$$

10

Functional Integral Representation of Quantum Field Theory

In theoretical physics, Fourier transformations have always played an important role in yielding complementary insights into mathematical structures. This is also true for generating functionals.

10.1 Functional Fourier Transform

Our goal is to study the functional Fourier transform of the generating functional $Z[j]$ of a scalar field theory. This will be written as

$$\tilde{Z}[\phi] \equiv \int \mathcal{D}j(x) Z[j] e^{-i\int d^Dx\, j(x)\phi(x)} \tag{10.1}$$

where the symbol $\int \mathcal{D}j(x)$ is called a *functional integral.*

The associated mathematics is an own discipline and discussed in many textbooks.[1] Functional integrals can be used to represent physical amplitudes without the use of operators in terms of fluctuating time dependencies of dynamical variables $q(t)$. They are defined by grating space-time into a fine lattice. For every coordinate x^μ, there we introduce discrete lattice points

$$x^\mu \to x^\mu_n \equiv n\epsilon, \quad n = 0,\ \pm 1,\ \pm 2,\ \pm 3, \tag{10.2}$$

with a very small ϵ. Then we may write

$$\int d^Dx\, j(x)\phi(x) = \epsilon^D \sum_n j(x_n)\phi(x_n) \equiv \epsilon^D \sum_n j_n \phi_n \tag{10.3}$$

where n is to be read as a four-index $(n_0,\ n_1,\ n_2,\ n_3)$, one for every coordinate. Now we define $\int \mathcal{D}j(x)$ as the infinite product of integrals over j_n at every point x_n

$$\int \mathcal{D}j(x) = \prod_n \int \frac{dj_n}{\sqrt{2\pi\epsilon^D}}. \tag{10.4}$$

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[1] See for example H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics,*
World Scientific Publishing Co., Singapore 1995, Second extended edition, pp. 1–850, and references therein.

One can operate with functional integrals very similar to ordinary integral. For example, the inverse Fourier transform reads

$$Z[j] = \int \mathcal{D}\phi(x) \tilde{Z}[\phi] e^{i\int d^D x\, j(x)\phi(x)}. \tag{10.5}$$

There are analogs of the usual δ-function:

$$\begin{aligned} \int \mathcal{D}j(x)\, e^{-i\int d^D x\, j(x)\phi(x)} &= \delta[\phi], \\ \int \mathcal{D}\phi(x)\, e^{i\int d^D x\, j(x)\phi(x)} &= \delta[j], \end{aligned} \tag{10.6}$$

called *δ-functional*. In the lattice approximation corresponding to (??), they are defined as infinite product of ordinary δ-functions

$$\delta[j] = \prod_n \sqrt{2\pi\epsilon^D}\,\delta(j_n). \tag{10.7}$$

They have the obvious property

$$\begin{aligned} \int \mathcal{D}\phi\, \delta[\phi] &= 1, \\ \int \mathcal{D}j\, \delta[j] &= 1. \end{aligned} \tag{10.8}$$

A useful notation for the measure of functional integrals (??) employs a continuously infinite product of integrals which must be imagined as the continuum limit of the lattice product (??). In this notation one writes $\int \mathcal{D}j(x)$ as

$$\int \mathcal{D}j(x) = \prod_x \int \frac{dj(x)}{\sqrt{2\pi}}, \tag{10.9}$$

and the associated δ-functionals as

$$\delta[j] = \prod_x \sqrt{2\pi}\,\delta(j(x)). \tag{10.10}$$

10.2 Gaussian Functional Integral

Up to now, not many functional integrals have been explicitly solved. The simplest nontrivial example is the Gaussian integral

$$\int \mathcal{D}j(x) e^{-\frac{i}{2}\int d^D x d^D x'\, j(x)M(x,x')j(x')}, \tag{10.11}$$

In the discretized form, this can be written as

$$\left[\prod_n \int \frac{dj_n}{\sqrt{2\pi\epsilon^D}}\right] e^{-i\epsilon^{2D}\sum_{n,m} j_n M_{nm} j_m}. \tag{10.12}$$

We may assume A to be a real symmetric functional matrix, since its antisymmetric part would not contribute to (??). Such a matrix may be diagonalized by a rotation

$$j_n \to j'_n = R_{nm} j_m \tag{10.13}$$

which leaves the measure of integration invariant

$$\frac{\partial\left(j_1, \dots, j_n\right)}{\partial\left(j'_1, \dots, j'_n\right)} = \det R^{-1} = 1. \tag{10.14}$$

Therefore we may factorize (??) into a product of Gaussian integrals,[2] which are easily calculated:

$$\prod_n \int \frac{dj'_n}{\sqrt{2\pi\epsilon}} e^{-\frac{i}{2}\epsilon^{2D}\sum_n j'_n M_n j'_n} = \prod_n \frac{1}{\sqrt{i\epsilon^D M_n}}. \tag{10.15}$$

Now, the product of M_n's is $\det M$, so that we obtain

$$\int \mathcal{D}j(x) e^{-\frac{i}{2}\int d^Dx\, d^Dx'\, j(x) M(x,x') j(x')} = \lim_{\epsilon\to 0}\left[\det\left(i\epsilon^D M\right)\right]^{-\frac{1}{2}}. \tag{10.16}$$

In order to calculate the determinant it is convenient to use the well-known matrix formula

$$(\det M)^{-\frac{1}{2}} = e^{-\frac{1}{2}\log\det M} = e^{-\frac{1}{2}\mathrm{tr}\log M} \tag{10.17}$$

and expand tr $\log(i\epsilon^D M)$ into power series

$$\mathrm{tr}\,\log\left[1 + \left(i\epsilon^D M - 1\right)\right] = -\mathrm{tr}\sum_{n=1}^{\infty}\frac{(-)^n}{n}\left(i\epsilon^D M - 1\right)^n \tag{10.18}$$

The advantage of this expansion is that the formula (??) can be taken to the continuum limit thus defining the *functional determinant* of the functional matrix $M(x,x')$ as

$$(\mathrm{Det}\, iM)^{-\frac{1}{2}} = e^{-\frac{1}{2}\log\det iM} = e^{-\frac{1}{2}\mathrm{Tr}\log iM} \tag{10.19}$$

via the corresponding expansion

$$\begin{aligned}\mathrm{Tr}\,\log iM &= \mathrm{Tr}\,\log\left[1 + (iM - 1)\right]\\ &= -\sum_{n=1}^{\infty}\frac{(-)^n}{n}\int d^Dx_1 \cdots d^Dx_n \left[iM(x_1,x_2) - \delta^{(D)}(x_1 - x_2)\right]\cdots\\ &\quad\times\left[iM(x_2,x_3) - \delta^{(D)}(x_2 - x_3)\right]\left[iM(x_n,x_1) - \delta^{(D)}(x_n - x_1)\right]\end{aligned} \tag{10.20}$$

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[2] Mathematically speaking, the Gaussian integrals with an imaginary exponent are more accurately called *Fresnel integrals*, but distinction is usually not made by field theorists.

We have used the fact that in (??), traces of powers of $\epsilon^D M$ are well-defined objects in the limit of infinitely fine gratings $\epsilon \rightarrow 0$:

$$\operatorname{tr} \epsilon^D M = \epsilon^D \sum_n M_{nn} \rightarrow \int d^D x \, M(x,x) \equiv \operatorname{Tr} M \tag{10.21}$$

$$\operatorname{tr} \left(\epsilon^D M\right)^2 = \epsilon^{2D} \sum_{nm} M_{nm} M_{mn} \rightarrow \int d^D x \, d^D x' \, M(x,x') M(x',x) \equiv \operatorname{Tr} M^2. \tag{10.22}$$

With this formula, we write the functional integral (??) as

$$\int \mathcal{D}j(x) e^{-\frac{i}{2}\int d^D x \, d^D x' \, j(x) M(x,x') j(x')} = (\operatorname{Det} iM)^{-\frac{1}{2}} . \tag{10.23}$$

This formula can be generalized to complex integration variables by separating the currents into real and imaginary parts, $j(x) = [j_1(x) + i j_2(x)]/\sqrt{2}$. Each integral gives the same functional determinant so that

$$\int \mathcal{D}j^*(x) \mathcal{D}j(x) e^{-i\int d^D x \, d^D x' \, j^*(x) M(x,x') j(x')} = (\operatorname{Det} iM)^{-1} , \tag{10.24}$$

where $M(x,x')$ is now an arbitrary *hermitian* matrix, and the measure of integration for complex $j(x)$ is defined as $\mathcal{D}j^*(x)\mathcal{D}j(x) \equiv \mathcal{D}j_1(x)\mathcal{D}j_2(x)$.

The *Gaussian functional integrals* in Eqs. (??) and (??) are can be used to calculate the Fourier transform of the generating functional $Z_0[j]$ of the free theory, which was defined in (5.761) and (5.764) and calculated explicitly for real scalar fields in Eq. (5.772),

$$Z_0[j] = e^{-\frac{1}{2}\int d^D x \, d^D x' \, j(x) G_0(x,x') j(x')}. \tag{10.25}$$

and for complex scalar fields in Eq. (5.772):

$$Z_0[j] = e^{-\int d^D x \, d^D x' \, j^*(x) G_0(x,x') j(x')}. \tag{10.26}$$

If we omit the spacetime indices, and use an obvious functional vector notation, the functional Fourier transform of $Z_0[j]$ can be written in the case of real fields as

$$A_0[\phi] = \int \mathcal{D}j e^{-\frac{i}{2} j^T \frac{1}{i} G_0 j + i j^T \phi}. \tag{10.27}$$

The exponent may be completed quadratically as

$$-\frac{i}{2}\left(j^T + iG_0^{-1}\phi\right)^T \frac{1}{i} G_0 \left(j + iG_0^{-1}\phi\right) + \frac{i}{2}\phi^T i G_0^{-1}\phi. \tag{10.28}$$

We now replace the variable $j + iG_0^{-1}\phi$ by j' which in each of the infinite integrals amounts only to a trivial shift of the center of integration. Thus

$$A_0[\phi] = \left(\int \mathcal{D}j' e^{-\frac{i}{2} j' \frac{1}{i} G_0 j'}\right) e^{\frac{i}{2}\phi^T i G_0^{-1}\phi}. \tag{10.29}$$

We can now apply formula (??) and find

$$A_0[\phi] = [\det(-iD)]^{\frac{1}{2}}\, e^{\frac{i}{2}\int d^Dx\, d^Dx'\, \phi(x)D(x,x')\phi(x')}, \tag{10.30}$$

where the functional matrix in the exponent is the inverse free-particle Green function:

$$D(x,x') = iG_0^{-1}(x,x') = (-\partial^2 - m^2)\delta^{(D)}(x-x'). \tag{10.31}$$

The determinant is a constant prefactor which does not depend on the field ϕ. We shall abbreviate it as a normalization factor

$$\mathcal{N} = [\det(-iD)]^{1/2} = (\operatorname{Det} G_0)^{-1/2}. \tag{10.32}$$

Using the explicit form (??), we can rewrite (??) after a partial integration of the derivative term as

$$A_0[\phi] = \mathcal{N}e^{i\int d^Dx\left[\frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2\right]} = \mathcal{N}e^{i\int d^Dx \mathcal{L}_0(\phi,\partial\phi)}. \tag{10.33}$$

Thus the Fourier-transformed generating functional is, up to the normalization factor $\mathcal{N}$, just the exponential of the classical action under consideration.

By Fourier-transforming (??), we undo the first transformation and return to the generating functional $Z_0[j]$, thereby obtaining a functional integral representation for the generating functional

$$Z_0[j] \;=\; \mathcal{N}\int \mathcal{D}\phi(x) e^{i\int d^Dx\,[\mathcal{L}_0(\phi,\partial\phi)+j(x)\phi(x)]}. \tag{10.34}$$

The functional integral over the ϕ-field is defined as in (??) by the product of integrals

$$\int \mathcal{D}\phi(x) = \prod_n \int \frac{d\phi_n}{\sqrt{2\pi\epsilon^D}}. \tag{10.35}$$

Let us check the normalizaion of (??). At zero source, $Z_0[j]$ has to be equal to unity [recall (??)]. This is ensured if

$$\mathcal{N}^{-1} = (\operatorname{Det} G_0)^{1/2} = \left[\int \mathcal{D}\phi e^{i\int d^Dx\, \mathcal{L}_0(\phi,\partial\phi)}\right]. \tag{10.36}$$

Indeed, by rewriting the right-hand side as

$$\left\{\int \mathcal{D}\phi(x) e^{i\int d^Dx\left[\frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2\right]}\right\} = \int \mathcal{D}\phi e^{i\int d^Dx\, \phi(x)D(x,x')\phi(x')}, \tag{10.37}$$

we can apply the Gaussian formula (??) and see that (??) is true due to (??). With (??) we can rewrite the expression (??) for the Fourier transform $A_0[\phi]$ as

$$A_0[\phi] = \frac{e^{i\int d^Dx\, \mathcal{L}_0(\phi,\partial\phi)}}{\int \mathcal{D}\phi(x) e^{i\int d^Dx\, \mathcal{L}_0(\phi,\partial\phi)}}. \tag{10.38}$$

This ratio is obviously normalized:

$$\int \mathcal{D}\phi A_0[\phi] = 1, \tag{10.39}$$

and has precisely the form of the quantum mechanical version (1.261) of the thermodynamical Gibbs distribution (1.259).

$$w_n \equiv Z_{\rm QM}^{-1}(t_b - t_a)e^{-iE_n(t_b-t_a)/\hbar}. \tag{10.40}$$

10.3 Functional Definition of Free Quantum Field Theories

Expression (??) with the normalization factor (??) may be used to *define* a free quantum field theory by functional integration,

$$Z_0[j] \;=\; ({\rm Det}\, G_0)^{-1/2} \int \mathcal{D}\phi(x) e^{i\int d^Dx\,[\mathcal{L}_0(\phi,\partial\phi)+j(x)\phi(x)]}, \tag{10.41}$$

and the integrand in Eq. (??) with $M(x,y) = iG_0(x,x')$ is the result of this functional integral:

$$Z_0[j] \;=\; e^{-\frac{1}{2}\int d^Dx d^Dx'\, j(x)G_0(x,x')j(x')}. \tag{10.42}$$

There exists useful formula for harmonically fluctuating fields which is encountered in many physical observables and which can be derived immediately from this. Consider the correlation function of two exponentials of a free field $\phi(x)$. Inserting into Eq. (??) a special current

$$j_{12}(x) = a\int d^Dx[a\phi(x-x_1) - b\phi(x-x_2)], \tag{10.43}$$

the partition function (??) reads

$$Z_0[j_{12}] \;=\; ({\rm Det}\, G_0)^{-1/2} \int \mathcal{D}\phi(x)\, e^{ia\phi(x_1)}e^{-ib\phi(x_2)}e^{i\int d^Dx\,[\mathcal{L}_0(\phi,\partial\phi)]}. \tag{10.44}$$

As such it coincides with the harmonic expectation value

$$\langle e^{ia\phi(x_1)}e^{-ib\phi(x_2)}\rangle. \tag{10.45}$$

Inserting the special current (??) into Eq. (??), we obtain the equation

$$\langle e^{ia\phi(x_1)}e^{-ib\phi(x_2)}\rangle = e^{-\frac{1}{2}\left[a^2G(x_1,x_1)-2abG(x_1,x_2)+b^2G(x_2,x_2)\right]} \tag{10.46}$$

In the brackest of the exponent we recognize the expectation values of pairs of fields

$$a^2\langle\phi(x_1)\phi(x_1)\rangle - 2ab\langle\phi(x_1)\phi(x_2)\rangle + b^2\langle\phi(x_2)\phi(x_2)\rangle, \tag{10.47}$$

such that we may write (??) also as

$$\langle e^{ia\phi(x_1)}e^{-ib\phi(x_2)}\rangle = \langle e^{ia\phi(x_1)-ib\phi(x_2)}\rangle = e^{-\frac{1}{2}\langle[a\phi(x_1)-b\phi(x_2)]^2\rangle}. \tag{10.48}$$

This result may also be derived for field operators using Wick's theorem of Section 5.12.1.

10.4 Interactions

Let us now include interactions. We have seen in Eq. (8.24) that the generating functional in the interaction picture [more precisely the functional $Z_D[j]$ of Eq. (8.22)] may simply be written as

$$Z[j]=e^{i\int d^Dx\,\mathcal{L}^{\rm int}(-i\delta/\delta j(x))}Z_0[j]. \tag{10.49}$$

This can immediately be Fourier-tranformed to

$$A[\phi]=\int\mathcal{D}je^{-i\int d^Dx\,j(x)\,\phi(x)}\left[e^{i\int d^Dx\,\mathcal{L}^{\rm int}(\phi)(-i\delta/\delta j)}Z_0[j]\right]. \tag{10.50}$$

Removing the second exponential by a partial functional integration, we obtain

$$\begin{aligned} A[\phi] &= e^{i\int d^Dx\,\mathcal{L}^{\rm int}(\phi)}\int\mathcal{D}je^{-i\int d^Dx\,j(x)\phi(x)}Z_0[j] \\ &= e^{i\int d^Dx\,\mathcal{L}^{\rm int}(\phi,\partial\phi)}\mathcal{N}e^{i\int d^Dx\,\frac{1}{2}\left[(\partial\phi)^2-m^2\phi^2\right]} \\ &= \frac{e^{i\int d^Dx\,\mathcal{L}(\phi,\partial\phi)}}{\int\mathcal{D}\phi(x)e^{i\int d^Dx\,\mathcal{L}_0(\phi,\partial\phi)}}. \end{aligned} \tag{10.51}$$

The Fourier transform of this expression renders the generalization of (??), the functional integral representation for the generating function of the interacting theory:

$$\begin{aligned} Z[j] &= \mathcal{N}\int\mathcal{D}\phi(x)e^{i\int d^Dx\,[\mathcal{L}(\phi,\partial\phi)+j(x)\phi(x)]} \\ &= \frac{\int\mathcal{D}\phi e^{i\int d^Dx\,[\mathcal{L}(\phi,\partial\phi)+j(x)\phi(x)]}}{\int\mathcal{D}\phi e^{i\int d^Dx\,\mathcal{L}_0(\phi,\partial\phi)(\phi)}}. \end{aligned} \tag{10.52}$$

This representation is to be compared with the perturbation theoretic formula of operator quantum field theory

$$Z[j]=\langle 0|Te^{i\int d^Dx\left[\mathcal{L}^{\rm int}(\phi)+j(x)\phi(x)\right]}|0\rangle, \tag{10.53}$$

where the symbol $\phi(x)$ denotes free-field operators, and the vacuum expectation value of products of these fields proceeds following Wick's theorem. In the new integral representations (??), (??), on the other hand, ϕ is a classical c-number object. All quantum properties of $Z[j]$ arise from the infinitely many integrals over ϕ, one at every space time point, rather than from field operators.

Note that in formula (??), the full action appears in the exponent, whereas in (??) only the interacting part appears.

In contrast to $A_0[\phi]$ of Eqs. (??) and (??), the amplitude for the interacting theory is no longer properly normalized. In fact, we know from the perturbative evaluation of (??) that it represents the sum of all vacuum diagrams. They were displayed in (8.69). Since the denominator does not normalize $A[\phi]$, it has become customary to drop it and work with the numerator only, and using the unnormalized

$$Z[j] \;=\; \int\mathcal{D}\phi(x)e^{i\int d^Dx\,[\mathcal{L}(\phi,\partial\phi)+j(x)\phi(x)]} \tag{10.54}$$

as the generating functional.

The normalization in (??) has an important advantage over the previous one in (??). In the euclidean formulation of the theory to be discussed in Section ??, it makes $Z[0]$ equal to the thermodynamic partition function of the system. In the quantum-mechanical version, there is only a trivial factor. This factor is simply an infinite product of factors $1/\sqrt{i}$, one for time point. This trivial factor is infinite (and thus in some sense nontrivial), but can easily be removed by redefining the measure of functional integration (??) as

$$\int \mathcal{D}\phi(x) = \prod_n \int \frac{d\phi_n}{\sqrt{2\pi i\epsilon}^D}. \tag{10.55}$$

Then the Gaussian integral formulas (??) and (??) become for real fields ϕ and a real symmetric functional matrix $M(x,x')$

$$\int \mathcal{D}\phi(x) e^{\frac{i}{2}\int d^Dx\, d^Dx'\, \phi(x)M(x,x')\phi(x')} = (\mathrm{Det}\, M)^{-\frac{1}{2}}, \tag{10.56}$$

and for complex fields $\phi = (\phi_1 + i\phi_2)/\sqrt{2}$, and a hermitian functional matrix $M(x,x')$

$$\int \mathcal{D}\phi^*(x)\mathcal{D}\phi(x) e^{i\int d^Dx\, d^Dx'\, \phi^*(x)M(x,x')\phi(x')} = (\mathrm{Det}\, M)^{-1}, \tag{10.57}$$

where $\mathcal{D}\phi^*(x)\mathcal{D}\phi(x) \equiv \mathcal{D}\phi_1(x)\mathcal{D}\phi_2(x)$.

In the limit of a free theory, $Z[0]$ is equal to the partition function of a set of harmonic oscillators of frequencies $\omega(\mathbf{k})$ for all momenta $\mathbf{k}$. This statement can be proved only in the lattice version of the theory. For the continuum formulas (??) and (??), this statement is nontrivial, since the determinants on the right-hand sides are infinite. However, we shall see in Section ??, Eqs. (??)–(??). that correct finite partition functions are obtained if the infinities are removed by the same method of dimensional regularization that was used before in Section 9.5 to remove divergences from Feynman integrals.

Even though the formulations (??) and (??) are completely equivalent there is an important advantage of the path integral formula (??). In some theories it may be difficult to find a canonically quantized set of free fields on which to construct an interaction representation for $Z[j]$ as in Eq. (??). The quantization of the photon field is an important example where it was quite hard to understand the Hilbert space. In particular, we encountered the problem that in the Gupta-Bleuler quantization scheme the vacuum energy contained the quanta of two unphysical polarization states of the photon. Within the functional approach, this will easily be explained in Chapter ??.

A second and very important advantage is the possibility of deriving from the representation (??) directly the Feynman rules without any knowledge of the Hilbert space. For this we simply take the non-quadratic piece of the action, which defines the vertices of the perturbation expansion, outside the functional integral as in (??), i.e., we rewrite (??) as:

$$Z[j] = e^{i\int d^Dx\, \mathcal{L}^{\mathrm{int}}(-i\delta/\delta j(x))} \mathcal{N} \int \mathcal{D}\phi(x) e^{i\int d^Dx\, [\mathcal{L}_0(\phi,\partial\phi)+j(x)\phi(x)]}. \tag{10.58}$$

Using (??), this reads more explicitly

$$Z[j] = e^{i\int d^Dx\,\mathcal{L}^{\rm int}(-i\delta/\delta j(x))}\mathcal{N}\int \mathcal{D}\phi(x)e^{\left[\frac{i}{2}\int d^Dx\,d^Dx'\,\phi(x)iG_0^{-1}(x,x')\phi(x')+j(x)\phi(x)\right]}. \tag{10.59}$$

A shift in the field variables to

$$\phi'(x) = \phi(x) + \int dy\,G_0(x,x')j(x'), \tag{10.60}$$

and a quadratic completion lead to

$$\begin{aligned} Z[j] = {} & e^{i\int d^Dx\,\mathcal{L}^{\rm int}(-i\delta/\delta j(x))}e^{-\frac{1}{2}\int d^Dx\,d^Dx'\,j(x)G_0(x,x')j(x')} \\ & \times\mathcal{N}\int \mathcal{D}\phi'(x)e^{\frac{i}{2}\int d^Dx\,d^Dx'\,\phi'(x)iG_0^{-1}(x,x')\phi'(x')}. \end{aligned} \tag{10.61}$$

The functional integral over the shifted field $\phi'(x)$ can now be performed with the help of formula (??), inserting there $M(x,x') = -iG_0(x,x')$. The result is, recalling (??),

$$\mathcal{N}\int \mathcal{D}\phi'(x)e^{\frac{i}{2}\int d^Dx\,d^Dx'\,\phi'(x)iG_0^{-1}(x,x')\phi'(x')} = \mathcal{N}[\text{Det}\,(-iG_0)]^{1/2}, \tag{10.62}$$

such that we find

$$Z[j] = \mathcal{N}[\text{Det}\,(-iG_0)]^{1/2}e^{i\int d^Dx\,\mathcal{L}^{\rm int}(-i\delta/\delta j(x))}e^{-\frac{1}{2}\int d^Dx\,d^Dx'\,j(x)G_0(x,x')j(x')}. \tag{10.63}$$

Expanding the prefactor in (??) in a power series yields all terms of the perturbation expansion (8.29), corresponding to the Wick contractions in Section 8.3.1, and to the accociated Fenyman diagrams. The free-field propagators is the functional inverse operator between the fields in the quadratic part of the Lagrangian. If this is written as

$$\frac{i}{2}\int d^Dx\,d^Dx'\,\phi(x)D(x,x')\phi(x') \tag{10.64}$$

then

$$G_0(x,x') = iD^{-1}(x,x'). \tag{10.65}$$

This formal advantage of obtaining perturbation expansions from the functional integral representations has far-reaching consequences. We have seen in Chapter 9 that the evaluation of the perturbation series proceeds most conveniently by Wick-rotating all energy integrations to run along the imaginary axes in the complex energy plane. In this way one avoids the singularities in the propagators at the physical particle energies. In Section 8.7, on the other hand, these singularities were shown to be responsible for the fact that particles leave a scattering region and form asymptotic states. Thus Wick-rotated perturbation expansions describe a theory which does not possess any particles states. In fact, they cannot be described by field operators and a Hilbert space.

These expansions can, however, be obtained from a simple modification of the above functional integral representation of the generating functional $Z[j]$. We simply perform the x-space version of the Wick-rotation in Fig. 5.2.

10.5 Euclidean Quantum Field Theory

In Eq. (5.127), we replaced in $D = 4$ spacetime dimensions the coordinates x^μ ($\mu = 0, 1, 2, 3$) by the *euclidean coordinates* $x_E^\mu = (x^1, \dots, x^3, x^4 = -ix^0)$. The same operation is done to the time x^0 in any dimensions. Under this, the action

$$\mathcal{A} \equiv \int d^Dx\, \mathcal{L}(\phi, \partial_E\phi) \equiv \int d^Dx \left\{ \left[\frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 \right] + \mathcal{L}^{\rm int}(\phi) \right\} \tag{10.66}$$

goes over into i times the *euclidean action*

$$\mathcal{A}_E = \int d^Dx_E \left\{ \left[\frac{1}{2}(\partial_E\phi)^2 + \frac{m^2}{2}\phi^2 \right] + \mathcal{L}^{\rm int}(\phi) \right\}. \tag{10.67}$$

The euclidean versions of the Gaussian integral formulas (??) and (??) are as

$$\int \mathcal{D}\phi(x) e^{-\frac{1}{2}\int d^Dx\, d^Dx'\, \phi(x) M(x,x')\phi(x')} = (\operatorname{Det} M)^{\mp\frac{1}{2}}, \tag{10.68}$$

and

$$\int \mathcal{D}\phi^*(x)\mathcal{D}\phi(x) e^{-\int d^Dx\, d^Dx'\, \phi^*(x) M(x,x')\phi(x')} = (\operatorname{Det} M)^{\mp 1}. \tag{10.69}$$

for complex fields $\phi = (\phi_1 + i\phi_2)/\sqrt{2}$, where $\mathcal{D}\phi^*(x)\mathcal{D}\phi(x) \equiv \mathcal{D}\phi_1(x)\mathcal{D}\phi_2(x)$.

The amplitude (??) becomes

$$A_E[\phi] = \frac{e^{-\int d^Dx_E\, \mathcal{L}_E(\phi,\partial\phi)}}{\int \mathcal{D}\phi(x) e^{-\int d^Dx_E\, \mathcal{L}_{E\,0}(\phi,\partial\phi)}}. \tag{10.70}$$

The normalized version of this

$$w[\phi] = \frac{e^{-\int d^Dx_E\, \mathcal{L}_E(\phi,\partial\phi)}}{\int \mathcal{D}\phi(x) e^{-\int d^Dx_E\, \mathcal{L}_E(\phi,\partial\phi)}} \tag{10.71}$$

represents the functional version of the proper quantum statistical Gibbs distribution corresponding to (??) [recall (1.259)]:

$$w_n = \frac{e^{-E_n/k_BT}}{\sum_n e^{-E_n/k_BT}}. \tag{10.72}$$

The functional integral representation for the unnormalized generating functional of all Wick-rotated Green functions corresponding to (??) is then

$$Z_E[j] \;=\; \int \mathcal{D}\phi(x) e^{-\int d^Dx_E\, [\mathcal{L}_E(\phi,\partial_E\phi) - j(x)\phi(x)]}. \tag{10.73}$$

The euclidean action corresponds to an energy of a field configuration. The integrand plays the role of a Boltzmann factor and gives the relative probability for this configuration to occur in a thermodynamic ensemble.

We now understand the advantage of working with the unnormalized functional integral: At zero external source, $Z_E[j]$ corresponds precisely to the thermodynamic partition function of the system. This will be seen explicitly in the examples in Section ??.

10.6 Functional Integral Representation for Fermions

If we want to use the functional technique to describe also the statistical properties of fermions, some modifications are necessary. Then the fields must be taken to be anticommuting c-numbers In mathematics, such objects form a Grassmann algebra G. If ξ, ξ' are real elements of G, then

$$\theta\theta' = -\theta'\theta. \tag{10.74}$$

A trivial consequence of this condition is that the square of each Grassmann element vanishes, i.e., $\theta^2 = 0$. If $\theta = \theta_1 + i\theta_2$ is a complex element of G, then $\theta^2 = -\theta^*\theta = -2i\theta_1\theta_2$ is nonzero, but $(\theta^*\theta)^2 = (\theta\theta)^2 = 0$.

All properties of operator quantum field theory for fermions can be derived from functional integrals if we find an appropriate extension of the integral formulas in the previous sections to Grassmann variables. Integrals are linear functional. For Grassmann variables, these are completely determined from the following basic integration rules:

$$\int \frac{d\theta}{\sqrt{2\pi}} \equiv 0, \quad \int \frac{d\theta}{\sqrt{2\pi}}\theta \equiv 1, \quad \int \frac{d\theta}{\sqrt{2\pi}}\theta^n \equiv 0,\ n > 1, \tag{10.75}$$

for real θ and

$$\int \frac{d\theta}{\sqrt{2\pi}} \equiv 0, \quad \int \frac{d\theta^*}{\sqrt{2\pi}}\theta \equiv 1, \quad \int \frac{d\theta}{\sqrt{2\pi}}\theta^* \equiv 1, \quad \int \frac{d\theta}{\sqrt{2\pi}}\frac{d\theta^*}{\sqrt{2\pi}}(\theta^*\theta)^n \equiv -\delta_{n1}, \tag{10.76}$$

for complex $\theta = (\theta_1 + i\theta_2)/\sqrt{2}$, where $d\theta d\theta^* = -id\theta_1 d\theta_2$.

Note that these integration rules make the linear operation of integration in (??) coincide with the linear operation of *differentiation*. A function $F(\theta)$ of a real Grassmann variable θ, is determined by only two parameters: the zeroth- and the first-order Taylor coefficients. Indeed, due to the property $\theta^2 = 0$, the Taylor series has only two terms $F(\theta) = F_0 + F'\theta$, where $F_0 = F(0)$ and $F' \equiv dF(\theta)/d\theta$. But according to (??), also the integral gives F':

$$\int \frac{d\theta}{\sqrt{2\pi}} F(\theta) = F'. \tag{10.77}$$

The coincidence of integration and differentiation has the important consequence that changes in integration variable do not transform with the Jacobian but with the inverse Jacobian:

$$\int \frac{d\theta}{\sqrt{2\pi}} = a \int \frac{d(a\theta)}{\sqrt{2\pi}}, \tag{10.78}$$

We shall use this transformation property below in Eq. (??).

As far as perturbation theory is concerned, it is sufficient to define only Gaussian functional integrals such as (??) and (??). In the discretized form, we may derive the formula

$$\prod_m \left[\int_{-\infty}^{\infty} \frac{d\theta_m}{\sqrt{2\pi i}}\right] \exp\left(\frac{i}{2}\sum_{k,l}\theta_k M_{kl}\theta_l\right) = (\det M)^{1/2}. \tag{10.79}$$

The right-hand side is the inverse of the bosonic result (??). In addition, there is an important difference: only the *antisymetric* part of the functional matrix contributes.

If the matrix M_{kl} is hermitian, complex Grassmann variables are necessary to produce a nonzero Gaussian integral. For these, we have

$$\prod_m \left[\int \frac{d\theta_m d\theta_m^*}{\sqrt{2\pi i}\sqrt{2\pi i}}\right] \exp\left(i\sum_{k,l}\theta_k^* M_{kl}\theta_l\right) = \det M, \tag{10.80}$$

the right-hand side being again the inverse of the corresponding bosonic result (??):

We first prove the latter formula. After bringing the matrix M_{kl} to diagonal form via a unitary transformation, we obtain the product of integrals

$$\prod_m \left[\int \frac{d\theta_m d\theta_m^*}{\sqrt{2\pi i}\sqrt{2\pi i}}\right] \exp\left(i\sum_n \theta_n^* M_n \theta_n\right). \tag{10.81}$$

Expanding the exponentials into a power series leaves only the first two terms since $(\theta_m^*\theta_m)^2 = 0$, so that the integral reduces to

$$\prod_m \int \frac{d\theta_m d\theta_m^*}{\sqrt{2\pi i}\sqrt{2\pi i}}(1 + i\theta_m^* M_m \theta_m). \tag{10.82}$$

Each of these integrals is performed via formulas (??), and we obtain the product of eigenvalues M_m, which is the determinant:

$$\prod_m M_m = \det M. \tag{10.83}$$

For real fermion fields, we observe that an arbitrary real antisymmetric matrix M_{kl} can always be brought by a real orthogonal transformation T to a canonical form $\mathbf{C}$ which is zero except for 2×2 matrices $c = i\sigma^2$ along the diagonal. Thus $M = T^T\mathbf{C}T$. The matrix $\mathbf{C}$ has a unit determinant so that $\det T = \det^{1/2}(M)$. Let $\theta_k' \equiv T_k\theta_l$, then the measure of integration in (??) changes according to (??) as follows:

$$\prod_k d\theta_k = \det T \prod_k d\theta_k'. \tag{10.84}$$

Applying now formulas (??), the Grassmann version of the functional integral (??) can be evaluated as follows:

$$\begin{aligned}\prod_m \left[\int \frac{d\theta_m}{\sqrt{2\pi i}}\right] \exp\left(i\sum_{k,l}\theta_k M_{kl}\theta_l\right) &= \det T \prod_m \left[\int \frac{d\theta_m'}{\sqrt{2\pi i}}\right] \exp\left(\sum_{kl}\theta_k' C_{kl}\theta_l'\right)\\ &= (\det M)^{1/2}\prod_n^\infty \left[\int \frac{d\theta_{2n}'}{\sqrt{2\pi}}\right] \frac{d\theta_{2n+1}'}{\sqrt{2\pi}}\left(1 + \theta_{2n}'\theta_{2n+1}'\right) = (\det iM)^{1/2},\end{aligned} \tag{10.85}$$

thus proving (??).

In the continuum limit, the result of this discussion can be summarized in an extension of the Gaussian functional integral formulas (??) and (??) to

$$\int \mathcal{D}\phi(x) e^{\frac{i}{2}\int d^Dx\, d^Dx'\, \phi(x)M(x,x')\phi(x')} = (\operatorname{Det} M)^{\mp\frac{1}{2}}\,, \tag{10.86}$$

where $M(x,x')$ is real symmetric or antisymmetric for bosons or fermions, respectively, and

$$\int \mathcal{D}\phi^*(x)\mathcal{D}\phi(x) e^{i\int d^Dx\, d^Dx'\, \phi^*(x)M(x,x')\phi(x')} = (\operatorname{Det} M)^{\mp 1}\,. \tag{10.87}$$

where the matrix is hermitian.

The functional integral formulation of fermions follows now closely that of bosons. For N relativistic real fermion fields χ_a obtain an amplitude $A[\chi_a]$ from the Fourier franform

$$A[\chi] = \int \mathcal{D}j(x) Z[j] e^{-i\int d^Dx\, j_a(x)\chi_a(x)}, \tag{10.88}$$

and find

$$A[\chi] = \frac{e^{i\int d^Dx\, \mathcal{L}(\chi,\partial\chi)}}{\left[\int \mathcal{D}\chi e^{i\int d^Dx\, \mathcal{L}_0(\chi,\partial\chi)}\right]}. \tag{10.89}$$

The functional

$$Z[j] = \mathcal{N} \prod_a \left[\int \mathcal{D}\chi_a\right] e^{i\int d^Dx\, \mathcal{L}(\chi,\partial\chi)}, \tag{10.90}$$

with a normalization factor

$$\mathcal{N}^{-1} = \prod_a \left[\int \mathcal{D}\chi_a\right] e^{i\int d^Dx\, \mathcal{L}_0(\chi,\partial\chi)}, \tag{10.91}$$

provides us with a functional integral representation of the generating functional of all Green functions.

An obvious extension of this holds for complex fermion fields In the case of a Dirac field, for example, where the sources j are commonly denoted by η, we obtain

$$Z[\eta,\bar\eta] = \mathcal{N} \int \mathcal{D}\psi\mathcal{D}\psi^* e^{i\int d^Dx \left[\bar\psi(i\partial\!\!\!/ - m)\psi + \mathcal{L}^{\rm int}(\psi) + \bar\eta\psi + \bar\psi\eta\right]} \tag{10.92}$$

with

$$\mathcal{N}^{-1} = \int \mathcal{D}\psi\mathcal{D}\psi^* e^{i\bar\psi(i\partial\!\!\!/ - m)\psi} = \operatorname{Det} iG_0^{-1}(x,x') = \operatorname{Det}(i\partial\!\!\!/ - m). \tag{10.93}$$

As in the boson case, we shall from now on work with the unnormalized functional without the factor $\mathcal{N}$,

$$Z[\eta,\bar\eta] = \int \mathcal{D}\psi e^{i\int d^Dx \left[\bar\psi(i\partial\!\!\!/ - m)\psi + \mathcal{L}^{\rm int}(\psi) + \bar\eta\psi + \bar\psi\eta\right]}, \tag{10.94}$$

which has also her the advantage that the euclidean version of $Z[0,0]$ becomes directly the thermodynamic partition function of the system.

The functional representations of the generating functionals can of course be continued to a euclidean form as in Section ??, thereby replacing operator quantum physics by statisticla physics. The corresponding Gaussian formulas for boson and fermion fields are the obvious generalization of Eqs. (??) and (??):

$$\int \mathcal{D}\phi(x) e^{-\frac{1}{2}\int d^Dx\, d^Dx'\, \phi(x) M(x,x')\phi(x')} = (\mathrm{Det}\, M)^{\mp\frac{1}{2}}, \tag{10.95}$$

and

$$\int \mathcal{D}\phi(x)\mathcal{D}\phi^*(x) e^{-\int d^Dx\, d^Dx'\, \phi^*(x) M(x,x')\phi(x')} = (\mathrm{Det}\, M)^{\mp 1}. \tag{10.96}$$

The euclidean version of the generating functional (??) renders all Wick-rotated Green functions.

10.7 Relation Between $Z[j]$ and Partition Function

The introduction of the unnormalized functional integral representation (??) for $Z[j]$ was motivated by the fact that in the euclidean version (??), $Z[0]$ is equal to the thermodynamic partition function of the system, up to a trivial factor. Let us verify this for a free field theory in $D = 1$ dimension. Then $Z_E[0]$ of Eq. (??) becomes

$$Z_\omega = \int \mathcal{D}x \exp\left\{-\int_0^\beta d\tau \left[\frac{1}{2}\dot{x}^2(\tau) + \frac{\omega^2}{2}x^2(\tau)\right]\right\}, \tag{10.97}$$

For $D = 1$. the fields $\phi(\tau)$ may be interpreted as paths $x(\tau)$ in imaginary time $\tau = -it$, and we have changed the notation accordingly. In the exponent, we recognize the euclidean version

$$\mathcal{A}_E = \int_0^\beta d\tau \left[\frac{1}{2}\dot{x}^2(\tau) + \frac{\omega^2}{2}x^2(\tau)\right] \tag{10.98}$$

of the action of the harmonic oscillator:

$$\mathcal{A} = \int_{t_a}^{t_b} dt \left[\frac{1}{2}\dot{x}^2(t) - \frac{\omega^2}{2}x^2(t)\right], \tag{10.99}$$

for $t_b - t_a = -i\hbar\beta = -i\hbar/k_BT$. Thus Z_ω is a quantum-statistical *path integral* for a harmonic oscillator. The measure of path integration is defined on lattice of points on the τ-axis $\tau_n = n\epsilon$ with $n = 0, \dots, N+1$ as (??):

$$\int \mathcal{D}x(\tau) = \prod_{n=0}^{N} \int \frac{dx_n}{\sqrt{2\pi\epsilon}}. \tag{10.100}$$

where $x_n \equiv x(\tau_n)$ and $N+1 = \hbar\beta/\epsilon$. For a finite τ-interval $\hbar\beta$, the paths have to satisfy periodic boundary conditions

$$x(\hbar\beta) = x(0), \tag{10.101}$$

as a reflection of the quantum-mechanical trace. On the τ-lattice, this implies $x_{N+1} = x_0$, and the action becomes

$$\mathcal{A}_E^N = \frac{1}{2}\epsilon \sum_{n=1}^{N+1} \left[\frac{(x_n - x_{n-1})^2}{\epsilon^2} + \omega^2 x_n^2 \right]. \tag{10.102}$$

This can be rewritten as

$$\mathcal{A}_E^N = \frac{1}{2\epsilon} \sum_{n=1}^{N+1} x_n(-\epsilon^2 \nabla\overline{\nabla} + \epsilon^2\omega^2) x_n. \tag{10.103}$$

where $\nabla\overline{\nabla}x$ denotes the lattice version of $\ddot{x}$. It may be represented as an $(N+1)\times(N+1)$-matrix

$$-\epsilon^2\nabla\overline{\nabla} = \begin{pmatrix} 2 & -1 & 0 & & \dots & 0 & 0 & -1 \\ -1 & 2 & -1 & & \dots & 0 & 0 & 0 \\ \vdots & & & & & & & \vdots \\ 0 & 0 & & 0 & \dots & -1 & 2 & -1 \\ -1 & 0 & 0 & & \dots & 0 & -1 & 2 \end{pmatrix}. \tag{10.104}$$

The Gaussian functional integral can now be evaluated using formula (??), and we obtain

$$Z_\omega = \det_{N+1}[-\epsilon^2\nabla\overline{\nabla} + \epsilon\omega^2]^{-1/2} \tag{10.105}$$

The determinant is calculated recursively,[3] with the result

$$Z_\omega = \frac{1}{2\sinh(\hbar\tilde{\omega}\beta/2)}, \tag{10.106}$$

with the auxiliar frequency

$$\tilde{\omega} \equiv \frac{2}{\epsilon}\text{arsinh}\frac{\omega\epsilon}{2}. \tag{10.107}$$

In the continnum limit $\epsilon \to 0$, the frequency $\tilde{\omega}$ goes against ω, and Z_ω becomes

$$Z_\omega = \frac{1}{2\sinh(\hbar\omega\beta/2)}. \tag{10.108}$$

Expanding this as

$$Z_\omega = e^{-\hbar\omega/2k_BT} + e^{-3\hbar\omega/2k_BT} + e^{-5\hbar\omega/2k_BT} + \dots \quad , \tag{10.109}$$

---

[3] See Section 2.12 of the textbook in Footnote ??.

this is the quantum statistical partition function of the harmonic oscillator, as we wanted to prove. The ground state has a nonzero energy, as observed in the operator discussion in Chapter 5.31.

For the quantum-mechanical version of the functional integral (??)

$$Z_\omega = \int \mathcal{D}x \exp\left\{ i \int_{t_a}^{t_b} dt \left[\frac{1}{2}\dot{x}^2(t) - \frac{\omega^2}{2} x^2(t) \right] \right\}, \tag{10.110}$$

we obtain with the measure of functional integration (??),

$$\int \mathcal{D}x(t) = \prod_{n=0}^{N} \int \frac{dx_n}{\sqrt{2\pi i \epsilon}}, \tag{10.111}$$

via the Gaussian integral formula (??) the result

$$Z_\omega = \det{}_{N+1}[-\epsilon^2 \nabla\overline{\nabla} - \epsilon\omega^2]^{-1/2}. \tag{10.112}$$

Thus we only have to replace $\omega \to i\omega$ in (??)–(??). In the continnum limit, we therefore obtain

$$Z_\omega = \frac{1}{2\sin(\hbar\omega\beta/2)}. \tag{10.113}$$

We end this section by mentioning that the path integral representation of the partition function (??) with the integration measure (??) can obtained from a euclidean phase space path integral [4]

$$Z_\omega = \int\int \mathcal{D}x(\tau) \frac{\mathcal{D}p(\tau)}{2\pi\hbar} \exp\left\{ \int_0^\beta d\tau \left[ip\dot{x} - \frac{1}{2}p^2 - \frac{\omega^2}{2}x^2 \right] \right\}, \tag{10.114}$$

by going to a τ-lattice and integrating out the momentum variables. The momentum integrals give the factors $\sqrt{2\pi\epsilon}$ in the denominators of the measure (??). In the quantum-mechanical version of (??)

$$Z_\omega = \int\int \mathcal{D}x(t) \frac{\mathcal{D}p(t)}{2\pi\hbar} \exp\left\{ i \int_{t_a}^{t_b} dt \left[p\dot{x} - \frac{1}{2}p^2 - \frac{\omega^2}{2}x^2 \right] \right\}, \tag{10.115}$$

they p-integrals produce the denominators containing the factors $\sqrt{i}$ in the measure (??).

The measure of funtional integration on the τ-lattice

$$\prod_{n=0}^{N} \left[\int_{-\infty}^{\infty} dx_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right] \tag{10.116}$$

---

[4] For a detailed discussion of the measure see Chapters 2 and 7 in the textbook on path integrals quoted in Footnote ??.

is the obvious generalization of the classical statistical weight in phase space

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \tag{10.117}$$

to fluctuating paths with many variables $x_n = x(\tau_n)$.

For completeness, we write down the free energy $F_\omega = -\beta \log Z_\omega$ associated with the partition function (??):

$$F_\omega = \frac{1}{\beta} \log[2\sinh(\hbar\omega\beta/2)] = \frac{\hbar\omega}{2} + \frac{1}{\beta}\log(1 - e^{-\beta\hbar\omega}). \tag{10.118}$$

At zero temperatures, only the ground-state oscillations contribute.

The detailed time-sliced calculation of the partition functions has to be compared with the formal evaluation of the partition function (??) according to formula (??), which would yield

$$\begin{aligned} Z_\omega &= \int \mathcal{D}x(\tau) \exp\left\{-\int_0^\beta d\tau \left[\frac{1}{2}\dot{x}^2(\tau) + \frac{\omega^2}{2}x^2(\tau)\right]\right\} \\ &= \text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2).. \end{aligned} \tag{10.119}$$

In this continnum formulation, the right-hand side is at first meaningless. It differs from the results obtained by proper time-sliced calculation (??)–(??) by a temperature-dependent infinite overall factor. To see what this factor is we note that for periodic boundary condition (??), the eigenvectors of the matrix $-\partial_\tau^2 + \omega^2$ are $e^{-i\omega_m\tau}$ with eigenvalues $\omega_m^2 + \omega^2$. Since ω_m grows with m like m^2, the functional determinant $\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)$ is strongly divergent. Indeed, the bosonic lattice result (??) can only be obtained dividing out of this determinant an equally divergent ω-independent functional determinant and calculating the ratio

$$\frac{\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)}{\hbar\beta\text{Det}'^{-1/2}(-\partial_\tau^2)}. \tag{10.120}$$

The prime in the denominator indicates that the zero-frequency ω_0 must be omitted to obtain a finite result. The factor $1/\hbar\beta)$ is the regularized contribution of the zero frequency. This follows from a simple integral consideration. An integral

$$\int_{-b/2}^{b/2} \frac{dx}{\sqrt{2\pi}} e^{-\omega^2 x^2/2} \tag{10.121}$$

gives $1/\omega$ only for finite $\omega(\gg 1/b)$. If $\omega \to 0$, it gives $b/\sqrt{2\pi}$. In the path integral, the zero mode is associated with the fluctuations of the average the path $x(\tau)$. To indicate this origin of the factor $\hbar\beta$ in the ratio (??), we may write (??) as

$$\frac{\text{Det}^{-1/2}(-\partial_\tau^2 + \omega^2)}{\text{Det}_R^{-1/2}(-\partial_\tau^2)}, \tag{10.122}$$

where the subscript R indicates the above regularization.

The ratio (??) is calculated via the product of eigenvalues:

$$\frac{\mathrm{Det}^{-1/2}(-\partial_\tau^2+\omega^2)}{\hbar\beta\mathrm{Det}'^{-1/2}(-\partial_\tau^2)}=\frac{1}{\hbar\beta\omega}\prod_{m>0}\frac{\omega_m^2}{\omega_m^2+\omega^2}. \tag{10.123}$$

The product can be found in tables:[5]

$$\prod_{m\neq 0}\frac{\omega_m^2}{\omega_m^2+\omega^2}=\frac{\hbar\beta\omega/2}{\sinh(\hbar\beta\omega/2)}, \tag{10.124}$$

so that (??) is equal to $1/2\sinh(\hbar\beta\omega/2)$, and the properly renormalized partition function (??) yields the lattice result (??).

In a lattice calculation, the determinant $\mathrm{Det}_R^{-1/2}(-\partial_\tau^2)$ for $\beta\rightarrow\infty$ is equal to unity.

It is curious to see that a formal evaluation of the functional determinant via the analytic regularization procedure of Sections 5.10 and 9.5 is indifferent to this denominator, and produces precisely the same result from the formal expression (??) as from the proper lattice calculation. Recalling formula (9.133) and setting $D=1$, we find

$$\begin{aligned}\mathrm{Det}^{-1/2}(-\partial_\tau^2+\omega^2) &= \exp\left\{-\frac{1}{2}\mathrm{Tr}\,\log(-\partial_\tau^2+\omega^2)\right\}\\ &= \exp\left\{-\frac{1}{2}\beta\hbar\int\frac{d\omega'}{2\pi}\log(\omega'^2+\omega^2)\right\}=e^{-\beta\frac{\hbar\omega}{2}}.\end{aligned} \tag{10.125}$$

The exponent gives is precisely the free energies in at zero temperatures in Eq. (??).

We now admit a finite temperatures. Then we have to replace the integral over ω' by a sum over Matsubara frequencies (2.375), and evaluate

$$\frac{1}{\hbar\beta}\sum_m\log(\omega_m^2+\omega^2)=\int\frac{d\omega'}{2\pi}\log(\omega'^2+\omega^2)+\left(\frac{1}{\hbar\beta}\sum_m-\int\frac{d\omega_m}{2\pi}\right)\log(\omega_m^2+\omega^2). \tag{10.126}$$

In contrast to the first term whose evaluation required the analytic regularization, the second term is finite. It can be rewritten as

$$-\left(\frac{1}{\hbar\beta}\sum_m-\int\frac{d\omega_m}{2\pi}\right)\int_{\omega^2}^{\infty}d\omega'^2\frac{1}{\omega_m^2+\omega'^2}. \tag{10.127}$$

Recalling the summation formula (2.384), this becomes

$$\begin{aligned}-\int_{\omega^2}^{\infty}\frac{d\omega'^2}{2\omega'}\left[\left\{\begin{array}{c}\coth(\hbar\beta\omega'/2)\\ \tanh(\hbar\beta\omega'/2)\end{array}\right\}-1\right] &= \pm\int_{\omega^2}^{\infty}\frac{d\omega'^2}{2\omega'}\frac{2}{e^{\beta\hbar\omega'}\mp 1}\\ &= k_BT\,2\log(1\mp e^{-\beta\hbar\omega}).\end{aligned} \tag{10.128}$$

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[5] I.S. Gradshteyn and I. M. Ryzhik, op. cit., Formula 1.431.2: $\sinh x=\prod_{m=1}^{\infty}(1+x^2/m^2\pi^2)$.

For later applications, we have treated also the case of fermionic Matsubara frequencies (the lower case). Together with the zero-temperature result (??), we find at any temperature

$$\begin{aligned} Z_\omega &= e^{-\beta F_\omega} = \mathrm{Det}^{-1/2}(-\partial_\tau^2+\omega^2) = \exp\left\{-\frac{1}{2}\mathrm{Tr}\,\log(-\partial_\tau^2+\omega^2)\right\} \\ &= \exp\left\{-\left[\beta\frac{\hbar\omega}{2}+\log(1-e^{-\beta\hbar\omega})\right]\right\}, \end{aligned} \tag{10.129}$$

in agreement with (??).

10.8 Bosons and Fermions in a Single State

The discussion in the last section cannot be taken over to fermionic variables $x(\tau)$ since in this case the action (??) vanishes identically, due to the symmetry of the functional matrix $D(\tau,\tau')=(-\partial_\tau^2+\omega^2)\delta(\tau-\tau')$. A fermionic version of the above path integral can only be introduced within the canonical formulation (??) of the harmonic path integral. With the help of a canonical transformation

$$a^\dagger=\sqrt{1/2\hbar\omega}(\omega x-ip),\quad a=\sqrt{1/2\hbar\omega}(\omega x+ip), \tag{10.130}$$

this may be transformed into the action

$$\mathcal{A}_{\omega\,\mathrm{QM}}=\int_{t_a}^{t_b}d\tau\,(a^*i\partial_t a-\omega a^*a). \tag{10.131}$$

A canonical quantization with commutation and anticommutation rules

$$\begin{aligned} [\hat a(t),\hat a^\dagger(t)]_\mp &= 1, \\ [\hat a^\dagger(t),\hat a^\dagger(t)]_\mp &= 0, \\ [\hat a(t),\hat a(t)]_\mp &= 0. \end{aligned} \tag{10.132}$$

produces a second-quantized Hilbert space of the type discussed in Chapter 2. Since $a^\dagger(t), a(t)$ carry no space variable, they desribe Bose and Fermi particles at a single point.

The path integral representation of the quantum-mechanical partition function of this system is

$$Z_{\omega\,\mathrm{QM}}\equiv\int\frac{\mathcal{D}a(t)\mathcal{D}a^*(t)}{2\pi}e^{i\mathcal{A}_{\omega\,\mathrm{QM}}}. \tag{10.133}$$

The measure of integration is

$$\int\!\!\int\frac{\mathcal{D}a^*\mathcal{D}a}{2\pi}\equiv\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathcal{D}\,a_1\mathcal{D}\,a_2}{2\pi}, \tag{10.134}$$

where $a=(a_1+ia_2)/\sqrt{2}$, is directly obtained from the canonical measure of path integration in (??).

At a euclidean time $\tau = -it$, the action of the free nonrelativistic field becomes

$$\mathcal{A}_\omega = \int_0^{\hbar\beta} d\tau \, (a^* \partial_\tau a + \omega a^* a), \tag{10.135}$$

and the thermodynamic partition function has the path integral representaion

$$Z_\omega \equiv \int \frac{\mathcal{D}a(\tau)\mathcal{D}a^*(\tau)}{2\pi} e^{-\mathcal{A}_\omega}. \tag{10.136}$$

In this formulation, there is no problem in trating simultaneously the case of bosons and fermions. We simply have to assume the fields $a(\tau), a^*(\tau)$ to be periodic and antiperiodic in the imaginary-time interval

$$a(\hbar\beta) = \pm a(0), \tag{10.137}$$

or in the sliced form

$$a_{N+1} = \pm a_0. \tag{10.138}$$

Using formula (??), the continuum partition function can be written as

$$\begin{aligned} Z_\omega &= \int \frac{\mathcal{D}a^*\mathcal{D}a}{2\pi} \exp\left[-\int_0^{\hbar\beta} d\tau \, (a^*\partial_\tau a + \omega a^* a)\right] \\ &= \operatorname{Det}^{\mp 1/2}(\partial_\tau + \omega). \end{aligned} \tag{10.139}$$

Contact with the previous oscillator calculation is established by observing that in the determinant, the operator $\partial_\tau + \omega$ can be replaced by the conjugate operator $-\partial_\tau + \omega$, since all eigenvalues come in complex-conjugate pairs, except for the $m = 0$ - value, which is real. Hence the determinant of $\partial_\tau + \omega$ can be substituted everywhere by

$$\det(\partial_\tau + \omega) = \det(-\partial_\tau + \omega) = \sqrt{\det(-\partial_\tau^2 + \omega^2)}, \tag{10.140}$$

In the boson case, we thus reobtain the result (??). In both cases, we may therefore write

$$Z_\omega = \operatorname{Det}^{\mp 1/2}(-\partial_\tau^2 + \omega^2). \tag{10.141}$$

The right-hand side was evaluate for bosons in Eqs. (??)–(??). Anticipating the present problem, we calculated the determinant up to Eq. (??) for bosons and fermions. The result for the two cases is then the obvious extension of (??):

$$\begin{aligned} Z_\omega &= e^{-\beta F_\omega} = \operatorname{Det}^{\mp 1/2}(-\partial_\tau^2 + \omega^2) = \exp\left\{\mp\frac{1}{2}\operatorname{Tr}\log(-\partial_\tau^2 + \omega^2)\right\} \\ &= \exp\left\{\mp\left[\beta\frac{\hbar\omega}{2} + \log(1 \mp e^{-\beta\hbar\omega})\right]\right\}. \end{aligned} \tag{10.142}$$

This can be written as

$$Z_\omega = \left\{ \begin{array}{c} [\sinh(\hbar\beta\omega/2)]^{-1} \\ \cosh(\hbar\beta\omega/2) \end{array} \right\} \quad \text{for} \quad \left\{ \begin{array}{c} \text{bosons,} \\ \text{fermions.} \end{array} \right\}. \tag{10.143}$$

For bosons, the physical interpretation of this expression was given after Eq. (??). In analogy we rewrite for fermions

$$Z_\omega = e^{\hbar\omega/2k_BT} + e^{-\hbar\omega/2k_BT}, \tag{10.144}$$

and see that the system has two states, one with no particle and one with one particle, where the no-particle state has a *negative* vacuum energy, as observed in the operator discussion in Chapter 2..

10.9 Free Energy for Free Scalar Fields

The results of the last section are easily applied to fluctuating scalar fields. Consider the free-field partition function

$$Z_0 \;=\; \int \mathcal{D}\phi(x) e^{-\int d^Dx \, \frac{1}{2}[(\partial\phi)^2 + m^2\phi^2]}, \tag{10.145}$$

which is of the general form (??) for $j = 0$. If the fields are decomposed into its spatial Fourier components in a finite box of volume V,

$$\phi(x) = \frac{1}{\sqrt{2V}} \sum_{\mathbf{k}} \int \left[e^{i\mathbf{kx}} \phi_{\mathbf{k}}(\tau) + \text{c.c.} \right], \tag{10.146}$$

the partition function becomes

$$Z_0 \;=\; \prod_{\mathbf{k}} \int \mathcal{D}\phi_{\mathbf{k}}(\tau) e^{-\int_0^{\hbar\beta} dt \, \frac{1}{2}\{|\dot\phi_{\mathbf{k}}(\tau)|^2 + \mathbf{k}^2|\phi_{\mathbf{k}}(\tau)|^2 + m^2|\phi_{\mathbf{k}}(\tau)|^2\}}. \tag{10.147}$$

For each $\mathbf{k}$, the functional integral is obviously the same as in (??), so that

$$Z_0 = \prod_{\mathbf{k}} Z_{\omega(\mathbf{k})}, \tag{10.148}$$

where $\omega(\mathbf{k}) \equiv \sqrt{\mathbf{k}^2 + m^2}$, and by (??)

$$Z_{\omega(\mathbf{k})} \;=\; \frac{1}{2\sinh[\hbar\omega(\mathbf{k})\beta/2]}. \tag{10.149}$$

For a real field $\phi(x)$, the anticommuting alternative cannot be accommodated into the functional integral (??). We must first go to the field-theoretic analog to the path integral in phase space

$$\begin{aligned} Z_0 = \int\int \mathcal{D}\phi(x) \frac{\mathcal{D}\pi(x)}{2\pi\hbar} \\ \times \exp\left\{ \int d^4x \left[i\pi(x)\partial_\mu\phi(x) - \frac{1}{2}\pi^2(x) - \frac{1}{2}(\boldsymbol{\nabla}\phi(x))^2 + \phi^2(x) \right] \right\}, \end{aligned} \tag{10.150}$$

where $\pi(x)$ are the canonical field momenta (5.1). After a Fourier decomposition (??) and a similar one for $\pi(x)$, we perform again a canonical tranformation corresponding to (??),

$$a^\dagger_{\mathbf{k}}(\tau) = \sqrt{1/2\hbar\omega}[\omega(\mathbf{k})\phi_{\mathbf{k}}(\tau) - i\pi_{\mathbf{k}}(\tau)], \;\; a_{\mathbf{k}}(\tau) = \sqrt{1/2\hbar\omega}[\omega(\mathbf{k})\phi_{\mathbf{k}}(\tau) + i\pi_{\mathbf{k}}(\tau)], \tag{10.151}$$

and arrive at the analog of (??):

$$\begin{aligned} Z_\omega &= \prod_{\mathbf{k}} \int \frac{\mathcal{D}a^*_{\mathbf{k}}\mathcal{D}a_{\mathbf{k}}}{2\pi} \exp\left[-\int_0^{\hbar\beta} d\tau\,(a^*_{\mathbf{k}}\partial_\tau a_{\mathbf{k}} + \omega a^*_{\mathbf{k}} a_{\mathbf{k}})\right] \\ &= \prod_{\mathbf{k}} \mathrm{Det}^{\mp 1/2}(\partial_\tau + \omega(\mathbf{k})). \end{aligned} \tag{10.152}$$

which can be evaluated as in (??) to

$$Z_\omega = \prod_{\mathbf{k}} \left\{ \begin{array}{c} \{2\sinh[\hbar\beta\omega(\mathbf{k})/2]\}^{-1} \\ 2\cosh[\hbar\beta\omega(\mathbf{k})/2] \end{array} \right\} \text{ for } \left\{ \begin{array}{l} \text{bosons,} \\ \text{fermions.} \end{array} \right\}. \tag{10.153}$$

The associated free energy is

$$F_0 = -\beta \log Z_0 = \pm \sum_{\mathbf{k}} \left\{ \frac{\omega(\mathbf{k})}{2} + \log\left[1 \mp e^{-\beta\hbar\omega(\mathbf{k})}\right] \right\}. \tag{10.154}$$

For a complex field, the canonical transformation is superfluous. The field in the partition function

$$Z_0 = \int \mathcal{D}\phi(x)\mathcal{D}\phi^*(x) e^{-\int d^D x \frac{1}{2}[\partial\phi^*\partial\phi + m^2\phi^*\phi]}, \tag{10.155}$$

can directly be assumed to be of the bosonic or fermionic type. A direct application of the Gaussian formula (??) yields

$$\begin{aligned} Z_\omega &= \prod_{\mathbf{k}} \mathrm{Det}\,(-\partial_\tau^2 + \omega^2(\mathbf{k}))^{\mp 1} \\ &= \prod_{\mathbf{k}} \left\{ \begin{array}{c} \{2\sinh[\hbar\beta\omega(\mathbf{k})/2]\}^{-2} \\ \{2\cosh[\hbar\beta\omega(\mathbf{k})/2]\}^{2} \end{array} \right\} \text{ for } \left\{ \begin{array}{l} \text{bosons,} \\ \text{fermions.} \end{array} \right\}, \end{aligned} \tag{10.156}$$

with a free energy twice as large as (??).

10.10 Gauge Fields and Gauge Fixing

The functional integral formalism developed in the last sections does not immediately apply to electromagnetism and any other gauge fields. There are subtleties which we are now going to discuss. These will lead to an explanation of the mistake in the vacuum energy observed in Eq. (5.491) when quantizing the electromagnetic field via the Gupta-Bleuler formalism. Consider a set of external electromagnetic currents described by the current density $j^\mu(x)$. Since charge is conserved, these satisfy

$$\partial_\mu j^\mu(x) = 0. \tag{10.157}$$

The currents are the sources of an electromagnetic fields $F_{\mu\nu}$ determined from the field equation (10.47):

$$\partial_\nu F^{\nu\mu}(x) = j^\mu(x), \tag{10.158}$$

if we employ natural units with $c = 1$. The action reads

$$\begin{aligned} \mathcal{A} &= \int d^4x \left[-\frac{1}{4} F_{\mu\nu}^2(x) - j^\mu(x) A_\mu(x) \right] \\ &= \int d^4x \left\{ \frac{1}{2} \left[\mathbf{E}^2(x) - \mathbf{B}^2(x) \right] - \left[\rho\phi(x) - \frac{1}{c} \mathbf{j} \cdot \mathbf{A}(x) \right] \right\}, \end{aligned} \tag{10.159}$$

The field strengths are the four-dimensional curls of the vector potential $A^\mu(x)$:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \tag{10.160}$$

so that they satisfy the Bianchi identity

$$\epsilon_{\mu\nu\lambda\kappa} \partial_\nu F_{\lambda\kappa} = 0. \tag{10.161}$$

The decomposition (??) is not unique. If we add to $A_\mu(x)$ the gradient of an arbitrary function $\Lambda(x)$,

$$A_\mu(x) \to A_\mu^\Lambda(x) = A_\mu(x) + \partial_\mu \Lambda(x) \tag{10.162}$$

then Λ does not appear in the field strengths if it satisfies Schwarz's integrability condition

$$(\partial_\mu \partial_\nu - \partial_\nu \partial_\mu) \Lambda(x) = 0, \tag{10.163}$$

i.e., if the derivatives in from of $\Lambda(x)$ commute. In the theory of partial differential equations, this is referred to as the *Schwarz integrability condition* for the function $\Lambda(x)$. In general, a function $\Lambda(x)$ which satisfies (??) in a simply-connected domain can be defined uniquely in this domain. This property makes (??) a *local gauge transformation*.

If the domain is multiply connected, there is more than one path along which to continue the function $\Lambda(x)$ from one spatial point to another and $\Lambda(x)$ becomes multi-valued. This happens, for example, if (??) is nonzero on a closed line in three-dimensional space in which case the set of paths between two given points decomposes into equivalence classes, depending on how often the closed line is being encircled. Each of these paths allows for another continuation of $\Lambda(x)$. By (??), such functions are *not* allowed in gauge transformations (??).

Let us now see how we can construct the generating functional of fluctuating free electromagnetic fields. in the presence of external currents $j_\mu(x)$. As in (??), we would like to calculate a functional integral, now in the unnormalized version corresponding to (??):

$$Z_0[j] = \int \mathcal{D}A^\mu(x) e^{i\int d^3x(-F_{\mu\nu}^2/4 - j_\mu A^\mu)}. \tag{10.164}$$

The $F_{\mu\nu}^2$-terms in the exponents can be partially integrated and rewritten as

$$-\frac{1}{4}\int d^4x F_{\mu\nu}^2 = \frac{1}{2}\int d^4x A^\mu(\partial^2 g_{\mu\nu} - \partial_\mu\partial_\nu)A^\nu. \tag{10.165}$$

Hence we can identify the functional matrix $D(x, x')$ in (??) as

$$D_{\mu\nu}(x, x') = (\partial^2 g_{\mu\nu} - \partial_\mu\partial_\nu)\delta^{(4)}(x - x'). \tag{10.166}$$

Recalling (??) [but in the unnormalized version, with the normalization factor $\mathcal{N}$ of Eq. (??) divided out] it appears, at first, as though the generating functional (??) should simply be equal to

$$Z_0[j] = (\mathrm{Det}\, G_{0\,\mu\nu})^{1/2} e^{-\frac{1}{2}\int d^4x d^4x' j_\mu(x) G_{0\,\mu\nu}(x,x') j_\mu(x')}, \tag{10.167}$$

where in analogy to (??)

$$G_{0\,\mu\nu}(x, x') = iD_{\mu\nu}^{-1}(x, x'), \tag{10.168}$$

and we have divided out a normalization factor $\mathcal{N} = (\mathrm{Det}\, G_{0\,\mu\nu})^{-1/2}$, since we are dealing with unnormalized version of $Z_0[j]$.

Unfortunately, the expression (??) is meaningless, since the inverse of the functional matrix (??) does not exist. In order to see this explicitly we diagonalize the functional part (i.e., the x, y-part) of $G_{0\,\mu\nu}(x, x')$ by going to the Fourier transform

$$D_{\mu\nu}(q) = -q^2 g_{\mu\nu} + q_\mu q_\nu. \tag{10.169}$$

For every momentum q, this matrix has obviously an eigenvector with zero eigenvalue, namely q_μ. This prevents us from inverting the matrix $D_{\mu\nu}(q)$. Correspondingly, when trying to form the inverse determinant of the functional matrix $D_{\mu\nu}$ in (??), we encounter an infinite number of infinities, one for every momentum q.

The difficulty can be resolved using the fact that the action (??) is gauge invariant. For $F_{\mu\nu}$ this is trivially true; for the source term $j^\mu(x)A_\mu(x)$ this is a consequence of current conservation. Indeed, if we change A_μ according to (??), the source term is changed by $\int d^4x\, j^\mu(x)\partial_\mu\Lambda(x)$. By a partial integration, this is equal to $-\int d^4x\, \partial_\mu j_\mu(x)(x)\Lambda(x)$, and this expression vanishes due to current conservation (??).

Because of this invariance, not all degrees of freedom over which are integrated over in the functional integral (??) are associated with a Gaussian integral. The fluctuations corresponding to pure gauge transformations which leave the exponent invariant. Since a path integral is a product of infinitely many integrals from minus to plus infinity, the gauge invariance of the integral produces an infinite product of infinite factors. This is precisely the infinity which occurs in the functional determinant origin of the infinities encountered when trying to calculate the inverse determinant of the functional matrix $D_{\mu\nu}(x,x')$.

This infinity must be avoided by restricting the functional integral to field fluctuations by specific gauge condition. The restriction is done by inserting into the integral *gauge-fixing functionals*, for example

$$\begin{array}{lll} F_1[A]=\delta[\partial_\mu A^\mu(x)], & \text{(Lorentz gauge)} & \\ F_2[A]=\delta[\boldsymbol{\nabla}\cdot\mathbf{A}(x)], & \text{(Coulomb gauge)} & \\ F_3[A]=\delta[A^0(x)], & \text{(Hamiltonian gauge)} & (10.170)\\ F_3[A]=\delta[A^3(x)], & \text{(axial gauge)} & \\ F_4[A]=\exp\left\{-\frac{i}{2\alpha}\int d^4x\,[\partial_\mu A^\mu(x)]^2\right\}. & & \end{array}$$

The first is a δ-functional enforcing the Lorentz gauge $\partial_\mu A^\mu(x)=0$. The second enforces the Coulomb gauge, the third corresponds to the axial gauge, and the fourth can be used to derive the Feynman diagrams of the Gupta-Bleuler quantization formalism, thereby correcting the mistake in the vacuum energy.

If we insert into any of these gauge-fixing functionals $F[A]$ the gauge-transformed vector potential (??), and integrate functionally over all $\Lambda(x)$, the integral receives a finite contribution for that gauge function $\Lambda(x)$ which enforces the desired gauge. The result is a gauge-invariant functionals of $A^\mu(x)$:

$$(10.171)$$

$$\Phi[A] \;=\; \int\mathcal{D}\Lambda F[A^\Lambda]=\int\mathcal{D}\Lambda F\delta[A+\partial\Lambda]. \qquad (10.172)$$

Explicitly, we find for the above cases (??):

$$\Phi_1[A] \;=\; \int\mathcal{D}\Lambda F_1[A^\Lambda]=\int\mathcal{D}\Lambda\delta[\partial_\mu A^\mu(x)+\partial^2\Lambda], \qquad (10.173)$$

$$\Phi_2[A] \;=\; \int\mathcal{D}\Lambda F_2[A^\Lambda]=\int\mathcal{D}\Lambda\delta[\boldsymbol{\nabla}\cdot\mathbf{A}(x)+\boldsymbol{\nabla}^2\Lambda], \qquad (10.174)$$

$$\Phi_3[A] \;=\; \int\mathcal{D}\Lambda F_2[A^\Lambda]=\int\mathcal{D}\Lambda\delta[\boldsymbol{\nabla}A^0(x)+\partial^0\Lambda], \qquad (10.175)$$

$$\Phi_4[A] \;=\; \int\mathcal{D}\Lambda F_3[A^\Lambda]=\int\mathcal{D}\Lambda\exp\left\{-\frac{i}{2\alpha}\int d^4x\,[\partial_\mu A^\mu+\partial^2\Lambda]^2\right\}. \qquad (10.176)$$

If we form the ratios $F_i[A]/\Phi_i[A]$, we obtain gauge fixing functionals which all yield unity if integrated over all gauge transformations. If any of these are inserted into the functional integral (??), they will all remove the gauge degree of freedom, and lead to a finite functional integral which is the same for each choice of $F_i[A]$.

Let us calculate the functionals $\Phi_i[A]$ explicitly. For $\Phi_{1,2,3}[A]$ we simply observe that the trivial identity for δ-functions

$$\delta(ax)=a^{-1}\delta(x), \qquad (10.177)$$

which is proved by multiplying both sides with a smooth function $f(x)$ and integrating over x, has a functional generalization

$$\delta[\mathcal{O}A]=\mathrm{Det}^{-1}\mathcal{O}\,\delta[A], \qquad (10.178)$$

where $\mathcal{O}$ is an arbitrary differential operator acting on the field $A^\mu(x)$. Hence we find immediately

$$\begin{aligned}
\Phi_1[A] &= \mathrm{Det}^{-1}(\partial^2), && (10.179)\\
\Phi_2[A] &= \mathrm{Det}^{-1}(\boldsymbol{\nabla}^2), && (10.180)\\
\Phi_3[A] &= \mathrm{Det}^{-1}(\partial^0), && (10.181)
\end{aligned}$$

The last functional $\Phi_4[A]$ is simply a Gaussian functional integral. The additive term $\partial_\mu A^\mu(x)$ can be removed by a trivial shift of the integration variable $\Lambda(x) \to \Lambda'(x) = \Lambda(x) - \partial_\mu A^\mu(x)/\partial^2$, under which the measure of integration remains invariant, $\mathcal{D}\Lambda = \mathcal{D}\Lambda'$. Using formula (??) we obtain

$$\Phi_4[A] = \mathrm{Det}^{-1/2}(\partial^4/\alpha). \tag{10.182}$$

The functional determinants Φ_i^{-1} are called *Fadeev-Popov determinants.*

The Fadeev-Popov determinants in the four examples happen to be *independent* of $A^\mu(x)$, so that we shall write them as Φ_i without arguments. This independence is a very useful property. Complications arising for A-dependent functionals $\Phi[A]$ will be illustrated below in an example.

We now study the consequences of inserting the gauge-fixing factors $F_i[A]/\Phi_i$. into the functional integrands (??). For $F_4[A]/\Phi_4$, the generating functional becomes

$$Z_0[j] = (\mathrm{Det}\, G_{0\,\mu\nu})^{1/2} \mathrm{Det}^{1/2}(\partial^4/\alpha) \int \mathcal{D}A_\mu(x) e^{i\int d^4x[-\frac{1}{4}F_{\mu\nu}^2 - \frac{1}{\alpha}(\partial^\mu A_\mu)^2 - j^\mu A_\mu]}. \tag{10.183}$$

The free-field action in the exponent can be written in the form

$$\mathcal{A} = \int d^4x \frac{1}{2}\left[-\left(\partial_\mu A_\nu\right)^2 + \left(1 - \frac{1}{\alpha}\right)\left(\partial^\mu A_\mu\right)^2\right]. \tag{10.184}$$

The associated Euler-Lagrange equation is

$$\partial^2 A^\mu - \left(1 - \frac{1}{\alpha}\right)\partial^\mu(\partial A) = 0, \tag{10.185}$$

which is precisely the field equation (5.366) of the covariant quantization scheme. With the additional term in the action, the matrix (??) becomes

$$D_{\mu\nu}(q) = -q^2\left[g_{\mu\nu} - \left(1 - \frac{1}{\alpha}\right)\frac{q_\mu q_\nu}{q^2}\right]. \tag{10.186}$$

This can be decomposed into projection matrices with respect to the subspaces transverse and longitudinal to the four-vector q^μ,

$$P^l_{\mu\nu}(q) = \frac{q_\mu q_\nu}{q^2}, \quad P^l_{\mu\nu}(q) = g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}, \tag{10.187}$$

as

$$D_{\mu\nu}(q) = -q^2\left[P^t_{\mu\nu}(q) + \frac{1}{\alpha}P^l_{\mu\nu}(q)\right]. \tag{10.188}$$

It is easy to verify that the matrices are really projections, since they satisfy

$$P^t_{\mu\nu}P^{t\nu}{}_\lambda = P^t_{\mu\nu}, \quad P^l_{\mu\nu}P^{l\nu}{}_\lambda = P^l_{\nu\lambda}, \quad P^t_{\mu\nu}P^{l\nu}{}_\lambda = 0. \tag{10.189}$$

A similar transverse projection appeared before in the three-dimensional subspace space [see (3.314), (10.6), and (10.76), (??) where the projection was indicated by a capital subscript T].

Due to the relations (??), there is no problem in inverting $D_{\mu\nu}(q)$, and we find the free photon propagator in momentum space

$$G_{0\,\mu\nu}(q) = iD^{-1}_{\mu\nu}(q) = -\frac{i}{q^2}[P^t_{\mu\nu}(q) + \alpha P^l_{\mu\nu}(q)] \tag{10.190}$$

$$= -\frac{i}{q^2}\left[g_{\mu\nu} - (1-\alpha)\frac{q_\mu q_\nu}{q^2}\right]. \tag{10.191}$$

For $\alpha = 0$, this is the propagator $G_{\mu\nu}$ derived in the Gupta-Bleuler canonical field quantization in Eq. (5.495), there obtained from canonical quantization rules with a certain filling of the vacuum with unphysical states.

Taking the Fadeev-Popov determinant Φ_4^{-1} of (??) into account, we obtain for the generating functional (??) the result:

$$Z[j] = [\mathrm{Det}\,(-iG_{0\,\mu\nu})]^{1/2}\mathrm{Det}^{\,1/2}(\partial^4/\alpha)e^{-\frac{1}{2}\int d^4x d^4x' j^\mu(x) G_{0\,\mu\nu}(x,x') j^\nu(x')} \tag{10.192}$$

Let us calculate the functional determinant $\mathrm{Det}\,G_{0\,\mu\nu}$. For this we take in the momentum representation (??) q^μ along the 0-direction and see that there are three spacelike eigenvectors of eigenvalues iq^2, and one timelike eigenvector of eigenvalue $i\alpha/q^2$, The total determinant is therefore

$$\mathrm{Det}\,(-iG_{0\,\mu\nu}) = \frac{1}{\mathrm{Det}\,(-\partial^2)^2\mathrm{Det}\,(\partial^4/\alpha)}. \tag{10.193}$$

The two prefactors together are therefore proportional to

$$[\mathrm{Det}\,(-iG_{0\,\mu\nu})]^{1/2}\mathrm{Det}^{\,1/2}(\partial^4/\alpha) \propto \frac{1}{\mathrm{Det}\,(-\partial^2)}. \tag{10.194}$$

Recalling the discussion from Eq. (??) to (??), we see that the associated free energy is

$$F_0 = -\beta \log Z_0 = 2\sum_{\mathbf{k}}\left\{\frac{\omega(\mathbf{k})}{2} + \log\left[1 - e^{-\beta\hbar\omega(\mathbf{k})}\right]\right\}. \tag{10.195}$$

It contains precisely the energy of the two physical transverse photons. The unphysical polarizations have been eliminated by the Fadeev-Popov determinant in (??).

We now understand why the Gupta-Bleuler formalism failed to get the correct vacuum energy in Eq. (5.491). It has no knowledge of the Fadeev-Popov determinant.

Taking current conservation into account, the exponent in (??) reduces to

$$j^\mu(x)G_{0\,\mu\nu}(x,x')j^\nu(x') = j^\mu(x)\frac{i}{\partial^2}j_\mu(x), \tag{10.196}$$

so that the generating functional becomes

$$Z[j] = \text{const} \times \text{Det}^{\,-1}(-\partial^2)e^{-\frac{1}{2}\int d^4x d^4x' j^\mu(x)(i/\partial^2)j_\mu(x')}, \tag{10.197}$$

where const is an infinite product of identical constant factors.

Let us see what happens in the other gauges (??). The results in the Lorentz gauge are immediately obtained by going to the limit $\alpha \to 0$ in the previous calculation. In this limit, the functional Φ_4 coincides with Φ_1, up to a trivial factor.

The Hamiltonian and the axial gauges are quite similar, so we may only discuss the one of them. In the Hamiltonian gauge where the Fadeev-Popov determinant is given by (??) we have, instead of the generating functional (??),

$$Z[j] = (\text{Det}\,G_{0\,\mu\nu})^{1/2}\text{Det}\,(\partial_0)e^{-\frac{1}{2}\int d^4x d^4x' j^i(x)G_{0\,ij\nu}(x,x')j^j(x')} \tag{10.198}$$

where the matrix $G_{0\,ij}(q)$ has only spatial entries, and is equal to

$$G_{0\,ij}(q) = iD^{-1}_{ij}(q) \tag{10.199}$$

with

$$D_{ij}(q) = q^2\delta_{ij} + q_iq_j \tag{10.200}$$

this being the spatial part of the 4×4-matrix (??). With the help of 3×3 projection matrices

$$P^T_{ij}(q) = \delta_{ij} - q_iq_j/\mathbf{q}^2 \tag{10.201}$$

$$P^L_{ij}(q) = q_iq_j/\mathbf{q}^2, \tag{10.202}$$

this can be decomposed as follows:

$$D_{ij}(q) = q^2P^T_{ij}(q) + q^{0\,2}P^L_{ij}(q). \tag{10.203}$$

The inverse of this is

$$D^{-1}_{ij}(q) = \frac{1}{q^2}P^T_{ij}(q) + \frac{1}{q^{0\,2}}P^L_{ij}(q) = \frac{1}{q^2}\left(\delta_{ij} - \frac{q_iq_j}{q^{0\,2}}\right). \tag{10.204}$$

In the exponent of (??) we have to evaluate $iD^{-1}_{ij}(q)$ between two conserved currents, and find

$$j^{i*}(q)G_{0\,ij}(q)j^j(q) = -\frac{i}{q^2}\left[\mathbf{j}^*(q)\cdot\mathbf{j}(q) - \frac{1}{q^{0\,2}}\mathbf{q}\cdot\mathbf{j}^*(q)\,\mathbf{q}\cdot\mathbf{j}(q)\right]. \tag{10.205}$$

Inserting the local current conservation law $\partial_\mu j^\mu(x) = 0$ in momentum space

$$\mathbf{q}\cdot\mathbf{j}(q) = q^0\,j^0(q), \tag{10.206}$$

we obtain

$$j^{i*}(q)G_{0\,ij}(q)j^j(q) = \frac{i}{q^2}\, j^{\mu *}(q)j_\mu(q). \tag{10.207}$$

Let us calculate the functional determinant $\mathrm{Det}\, G_{0\,\mu\nu}$ in this gauge. From (??) we see that $G_{0\,\mu\nu}$ has two eigenvectors of eigenvalue i/q^2, and one eigenvector of eigenvalue $-i/q^{0\,2}$. Hence:

$$\mathrm{Det}\, G_{0\,\mu\nu} = \frac{1}{\mathrm{Det}\,(-i\partial^2)^2 \mathrm{Det}\,(i\partial_0^2)}. \tag{10.208}$$

The two prefactors in (??) together are therefore proportional to

$$(\mathrm{Det}\, G_{0\,\mu\nu})^{1/2}\mathrm{Det}\,(\partial_0) \propto \frac{1}{\mathrm{Det}\,(-i\partial^2)}, \tag{10.209}$$

which is the same as (??).

Thus the generating functional (??) agrees with the previous one (??)

We leave it as an exercise to show that also the Coulomb gauge leads to the same result.

10.11 Nontrivial Gauge and Fadeev-Popov Ghosts

The Fadeev-Popov determinants in the above examples were all independent of the fields. As such they were irrelevant for the calculation of any Green function. This is not always true.

Consider the following nontrivial gauge-fixing functional

$$F[A] = \delta\left[(\partial A)^2 + gA^2\right]. \tag{10.210}$$

As in Eqs. (??)-(??), we calculate

$$\Phi[A] \;=\; \int \mathcal{D}\Lambda F[A^\Lambda] = \int \mathcal{D}\Lambda\; \delta[\partial A + gA^2 + \partial^2\Lambda + 2gA\partial\Lambda + g(\partial\Lambda)^2]. \tag{10.211}$$

This path integral can trivially be performed in analogy with the ordinary integral

$$\int dx\, \delta(ax + bx^2) = \frac{1}{a}, \tag{10.212}$$

and the result is

$$\Phi[A] = \mathrm{Det}\,(\partial^2 + 2gA_\mu\partial^\mu)^{-1}. \tag{10.213}$$

The generating functional is therefore

$$Z[j] \;=\; \int \mathcal{D}A^\mu \mathrm{Det}\,(\partial^2 + 2gA^\mu\partial_\mu)\; \delta[\partial_\mu A^\mu + gA^2] \exp\left[i\int d^4x \left(-\frac{1}{4}F_{\mu\nu}^2 - j_\mu A^\mu\right)\right]. \tag{10.214}$$

Contrary to the previous gauges, the determinant is no longer a trivial overall factor but depends now functionally on the field A^μ. It can therefore no longer be brought outside the functional integral.

There is a simple way of including its effect within the usual field-theoretic formalism. On e introduces an auxiliary *Fadeev-Popov ghost field.* We may consider the determinant as the result of a fluctuating complex fermion field c with a complex-conjugate c^*, and write

$$\mathrm{Det}\,(\partial^2 + 2gA^\mu\partial_\mu) = \int \mathcal{D}c^*\mathcal{D}c e^{-i\int d^4x(\partial c^*\partial c - 2gA^\mu c^*\partial_\mu c)}. \tag{10.215}$$

Note that the Fermi fields are necessary to produce the determinant in the numerator; a Bose field would have put it into the denominator. A complex field is taken to make the determinant appear directly rather than the square-root of it.

The ghost fields interact with the photon fields. This interaction is necessary in order to compensate for the interactions induced by the constraint $\delta[\partial A^\mu + gA^2]$ in the functional integral.

It is possible to exhibit the associated cancellations order by order in perturbation theory. For this we have to bring the integrand to a form in which all fields appear in the exponent. This can be achieved for the δ-functional by observing that the same representation (??) would be true with any other choice of gauge, say

$$\delta[\partial_\mu A^\mu(x) + gA^2(x) - \lambda(x)] \tag{10.216}$$

since this would lead to the same Fadeev-Popov ghost term (??). Therefore we can average over all possible functions $\lambda(x)$ with a Gaussian weight and replace (??) just as well by

$$\int \mathcal{D}\lambda e^{-\frac{i}{2}\int d^4x\lambda^2(x)}\,\delta[\partial_\mu A^\mu(x) + gA^2(x) - \lambda(x)]. \tag{10.217}$$

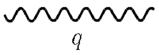
Now the generating functional has the form

$$Z[j] = \int \mathcal{D}A^\mu \int \mathcal{D}c^*\mathcal{D}c e^{i\int d^4x(\mathcal{L} - j^\mu A_\mu)} \tag{10.218}$$

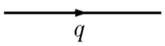
with a Lagrangian

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}^2 - \frac{1}{2\alpha}\left(\partial A + gA^2\right)^2 - \partial_\mu c^*\partial^\mu c + 2gA^\mu c^*\partial_\mu c. \tag{10.219}$$

The photon and ghost propagators are



$$\dot{A}_\mu(x)\dot{A}_\nu(0) = -\int \frac{d^4k}{(2\pi)^4} e^{-ikx}\frac{i}{k^2}\left[g_{\mu\nu} - (1-\alpha)\frac{k_\mu k_\nu}{k^2}\right], \tag{10.220}$$

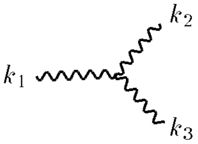


$$\dot{c}^*(x)\dot{c}(0) = -\int \frac{d^4q}{(2\pi)^4} e^{-iqx}\frac{i}{q^2}. \tag{10.221}$$

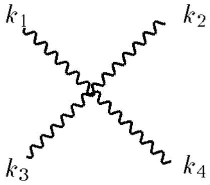
Contrary to the previous gauges, there are now photon-ghost and photon-photon interaction terms

$$-\frac{g}{\alpha}\partial_\mu A^\mu A^2-\frac{g^2}{2\alpha}\left(A_\mu^2\right)^2+2gA^\mu c^*\partial_\mu c \tag{10.222}$$

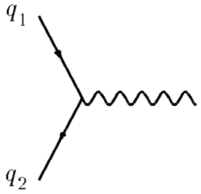
with the corresponding vertices



$$=\frac{2g}{\alpha}\left(g_{\mu_1\mu_2}k_{3\mu_3}+g_{\mu_2\mu_3}k_{1\mu_1}+g_{\mu_3\mu_1}k_{2\mu_2}\right)$$



$$=-\frac{4ig^2}{\alpha}\left(g_{\mu_1\mu_2}g_{\mu_3\mu_4}+g_{\mu_1\mu_3}g_{\mu_2\mu_4}+g_{\mu_1\mu_4}g_{\mu_2\mu_3}\right)$$



$$=-g\left(q_1+q_2\right)_\mu$$

It can be shown that the Fadeev-Popov ghost Lagrangian has the property of canceling all these unphysical contributions order by order in perturbation theory. We leave it as an exercise to show, for example, that there is no contribution of the ghosts to photon-photon scattering up to, say, second order in g, and that self-energy corrections to the photon propagator due to photon and ghost loops cancel exactly.

In the context of quantum electodynamics, there is little sense in using a gauge fixing term (??). The present discussion is, however, a useful warm-up exercise to gauge-fixing procedures in nonabelian gauge theories, where the Fadeev-Popov determinant will always be field dependent.

Of course, also the previous field-independent Fadeev-Popov determinants can be generated from fermionic ghost fields. The determinant Φ_4^{-1} in (??), for example, can be generated from a complex ghost field $c(x)$ and its complex conjugate c^* by a functional integral

$$\Phi_4^{-1}=\int\mathcal{D}c^*\mathcal{D}c\,e^{i\int d^4x\,\partial c^*\partial c/\sqrt{\alpha}}. \tag{10.223}$$

It should be pointed out that the sign of the kinetic term of these c-field Lagrangians are opposite to those of a normal field. If these fields were associated with particles, their anticommutation rules would carry the wrong sign and the states would have a negative norm. Such states are commonly referred to as *ghosts*, and this is the reason for the name of the fields c, c^*.

Note that the determinant cannot be generated by a real fermion field via a functional integral

$$\Phi_4^{-1}\overset{?}{=}\int\mathcal{D}c\,e^{-i\int d^4x\,\partial^2c\partial^2c/\alpha}. \tag{10.224}$$

The reason is that the differantial operator ∂^4 is a *symmetric* functional matrix, so that the exponent vanishes after diagonalization by an orthogonal tranformation.

In the language of ghost fields, the mistake in calculating the vacuum energy in Eq. (5.491) when quantizing the electromagnetic field via the Gupta-Bleuler formalism can be phrased as follows. When fixing the gauge in the action (5.361) by adding an Lagrangian density $\mathcal{L}_{\rm GF}$ (8.74), we must also add a ghost Lagrangian density

$$\mathcal{L}_{\rm ghost} = \partial c^* \partial c / \sqrt{\alpha}. \tag{10.225}$$

The ghost fields have to be quantized canonically, and the physical states must satisfy, beside the Gupta-Bleuler subsidiary condition in Eq. (5.487), the condition of being a vacuum to the ghost fields:

$$c|\psi_{\text{``phys''}}\rangle = 0. \tag{10.226}$$

The Fadeev-Popov formalism is extremely useful offering many other possibilities of fixing a gauge and performing the functional integral for the generating functional over all A^μ-components.

12

Formal Properties of Perturbation Theory

In Chapter 8 we have observed simple composition rules which help to construct all Feynman diagrams of a field theore from connectd diagrams which, in turn, can be decomposed in a simple way into one-particle irreducible ones, These composition rules can be derived by simple functional operations on appropriate generating functionals.

12.1 Connectedness Structure of Feynman Diagrams

In view of the applications to come, we write the action in a rather general form

$$\mathcal{A}[\varphi] = \mathcal{A}^0[\varphi] + \mathcal{A}^{\rm int}[\varphi] \tag{12.1}$$

with a free action

$$\mathcal{A}^0[\varphi] = \frac{1}{2}\int d^Dx'\, d^Dx\, \varphi(x) i G_0^{-1}(x',x)\varphi(x) \tag{12.2}$$

and an interaction

$$\begin{aligned}\mathcal{A}^{\rm int}[\varphi] &= -\frac{1}{3!}\int d^Dx_1 d^Dx_2 d^Dx_3 V_3\,(x_1,x_2,x_3)\varphi(x_1)\varphi(x_2)\varphi\,(x_3) \\ &\quad -\frac{1}{4!}\int d^Dx_1 d^Dx_2 d^Dx_3 d^Dx_4\, V_4(x_1,x_2,x_3,x_4)\varphi(x_1)\varphi(x_2)\varphi(x_3)\varphi(x_4).\end{aligned} \tag{12.3}$$

In the relativistic scalar theory discussed in the previous two chapters the operator iG_0^{-1} between the φ-fields had the specific form

$$iG_0^{-1}(x,x') = \delta^{(D)}(x-x')(-\partial^2 - m^2). \tag{12.4}$$

We shall find it convenient to introduce a short notation and write (12.2) as

$$\mathcal{A}^0[\varphi] = \frac{1}{2}\varphi i G_0^{-1}\varphi. \tag{12.5}$$

Here the fields are considered as vectors with continuous indices x, whereas $G_0^{-1}(x,x')$ is a corresponding matrix. Such objects will be referred to as functional vectors and matrices, respectively. This notation will permit an immediate adaptation of all formulas to be derived in this chapter to many different field theories. With x being considered as a functional index, V_3, and V_4 may be viewed as functional tensors which are symmetric in all indices. We can save many integral symbols by rewriting (12.3) in analogy with (12.5) short as

$$\mathcal{A}^{\rm int}[\varphi] = -\frac{1}{3!}V_3\varphi^3 - \frac{1}{4!}V_4\varphi^4, \tag{12.6}$$

where the successive contraction of the functional indices x is implied.

For the above general action and in this notation, the Heisenberg field operator φ satisfies an equation of motion

$$iG_0^{-1}\varphi + \frac{\delta\mathcal{A}^{\rm int}[\varphi]}{\delta\varphi} = 0. \tag{12.7}$$

or explicitly

$$iG_0^{-1}\varphi(x) - \frac{V_3}{2!}\varphi^2 - \frac{V_4}{3!}\varphi^3 = 0. \tag{12.8}$$

12.2 Functional Differential Equations

The operator equation (12.8) can be used to derive a differential equation for the generating functional $Z[j]$ of the theory defined in Eq. (5.760). In the functional vector notation introduced above we, shall write the generating functional as

$$Z[j] = \langle Te^{ij\varphi}\rangle. \tag{12.9}$$

In order to apply (12.8), we form the derivative

$$\frac{\delta}{i\delta j}Z[j] = \langle T\varphi e^{ij\varphi}\rangle \tag{12.10}$$

and multiply this by the functional matrix iG_0^{-1}. When passing iG_0^{-1} to the right of the time-ordering operator we generate the φ^2 and φ^3 terms of (12.8). These can also be obtained from higher derivatives $(\delta/\delta j)^2$, $(\delta/\delta j)^3$ applied to $Z[j]$. The passage of the time-ordering operator produces some additional terms in the same way as in the derivation of the equation for the Green functions in (5.40) (5.42). Its calculation requires the use of the canonical equal-time commutation rules. Since these are the same for interacting and free fields, we can evaluate them for the free fields and consider taking iG_0^{-1} to the right of the time-ordering operator in the free-field expression

$$iG_0^{-1}\frac{\delta}{i\delta j}Z_0[j]. \tag{12.11}$$

The free partition function was calculated in Section 5.14. In Eqs. (5.763) and (5.764)] we found

$$Z^0[j] = e^{-\frac{1}{2}jG_0j}. \tag{12.12}$$

satisfying the functional differential equation

$$iG_0 \frac{\delta}{i\delta j(x)} Z^0[j] + j(x) Z^0[j] = 0. \tag{12.13}$$

The generalization to the interacting case follows directly by adding the interaction terms of (12.8) expressed in terms of derivatives with respect to the current:

$$\left[iG_0^{-1} \frac{\delta}{i\delta j} - \frac{V_3}{2!} \left(\frac{\delta}{i\delta j} \right)^2 - \frac{V_4}{3!} \left(\frac{\delta}{i\delta j} \right)^3 + j \right] Z\left[j\right] = 0. \tag{12.14}$$

For the subsequent development it is useful to introduce the short-hand notation

$$\frac{\delta}{i\delta j} \frac{\delta}{i\delta j} \cdots \frac{\delta}{i\delta j} Z[j] = Z_{jj\dots j}[j], \tag{12.15}$$

with the arguments $x_1, \dots, x_n$ of the currents suppressed. Then we may write (12.14) as

$$iG_0^{-1} \frac{1}{i} Z_j - \frac{V_3}{2!} \frac{1}{i^2} Z_{jj} - \frac{V_4}{3!} \frac{1}{i^3} Z_{jjj} + jZ = 0 \tag{12.16}$$

This equation can be used to calculate $Z[j]$ recursively. We have seen, however, in the previously discussed example of φ^4-theory that $Z[j]$ is not a very economic quantitiy to deal with. Its expansion coefficients, the n-point Green functions, contain many disconnected pieces. A substantial simplification arises by going over to the functional $iW[j]$ defined by

$$iW[j] = \log Z[j]. \tag{12.17}$$

It serves as a generating functional for the connected part of the Green functions which are obtained from

$$G_{\mathrm{c}}^{(n)}(x_1, \dots, x_n) = \frac{\delta}{i\delta j(x_1)} \cdots \frac{\delta}{i\delta j(x_n)} iW[j]. \tag{12.18}$$

Using the differential equation (12.16) we are able to prove quite generally that these Green functions do deserve their name since their graphical representation consists only of connected diagrams. Moreover, the connected Green functions collect precisely all the connected diagrams in $G^{(n)}(x_1, \dots, x_n)$ and the full Green functions $G^{(n)}(x_1, \dots, x_n)$ can be recovered in a simple way from the connected ones $G_{\mathrm{c}}^{(n)}(x_1, \dots, x_n)$. Let us first prove this by deriving the general relationship between the two types of Green functions. This relationship serves to transform the functional differential equation (12.16) for $Z[j]$ into a more useful one for $W[j]$ which will enable us to prove the connectedness of the Green functions $G_{\mathrm{c}}^{(n)}(x_1, \dots, x_n)$.

12.3 Decomposition of Green Functions into Connected Green Functions

Using the exponential relation (12.17) between iW and Z we can now derive general relations between the n-point functions and the connected ones. For the one-point function we find

$$G^{(1)}(x) = Z^{-1}[j]\frac{\delta}{ij(x)}Z[j] = \frac{\delta}{\delta j}W[j] = G_{\rm c}^{(1)}(x). \tag{12.19}$$

Thus the one-point function, which represents the ground state expectation value of the field, is always connected:

$$\langle\varphi(x)\rangle \equiv G^{(1)}(x) = G_{\rm c}^{(1)}(x). \tag{12.20}$$

We may convince ourselves by drawing the Feynman diagrams corresponding to the formula

$$G^{(1)}(x) = \frac{\langle 0|T\varphi(x)e^{i\mathcal{A}^{[\varphi]}_{\rm int}+j\varphi}|0\rangle}{\langle 0|Te^{i\mathcal{A}_{\rm int}[\varphi]}|0\rangle} \tag{12.21}$$

that this is indeed true. All disconnected pieces cancel when forming the quotient.

Consider now the two-point function where

$$\begin{aligned} G^{(2)}(x_1,x_2) &= Z^{-1}[j]\frac{\delta}{i\delta j(x_1)}\frac{\delta}{i\delta j(x_2)}Z[j] \\ &= Z^{-1}[j]\frac{\delta}{i\delta j(x_1)}\left\{\left(\frac{\delta}{i\delta j(x_2)}iW[j]\right)Z[j]\right\} \\ &= Z^{-1}[j]\left\{\frac{1}{i}W_{j(x_1)j(x_2)} + W_{j(x_1)}W_{j(x_2)}\right\}Z[j] \\ &= G_{\rm c}^{(2)}(x_1,x_2) + G_{\rm c}^{(1)}(x_1)\,G_{\rm c}^{(1)}(x_2)\,. \end{aligned} \tag{12.22}$$

In addition to the connected diagrams with two ends there are two connected diagrams ending in a single line. These are absent in a pure φ^4-theory at $j=0$ if the ground state of the system is normal, a specification which we are going to understand only later when discussing phase transitions.

For the three-point function we find

$$\begin{aligned} G^{(3)}(x_1,x_2,x_3) &= Z^{-1}[j]\frac{\delta}{i\delta j(x_1)}\frac{\delta}{i\delta j(x_2)}\frac{\delta}{i\delta j(x_3)}Z[j] \\ &= Z^{-1}[j]\frac{\delta}{i\delta j(x_1)}\frac{\delta}{i\delta j(x_2)}\left\{\left[\frac{\delta}{i\delta(x_3)}iW[j]\right]Z[j]\right\} \\ &= Z^{-1}[j]\frac{\delta}{i\delta(x_1)}\left\{\left[\frac{1}{i}W_{j(x_2)k(x_3)} + W_{j(x_2)}W_{j(x_3)}\right]Z[j]\right\} \\ &= Z^{-1}[j]\left\{\frac{1}{i^2}W_{j(x_1)j(x_2)j(x_3)} + i\left(W_{j(x_1)}W_{j(x_2)j(x_3)} + W_{j(x_2)}W_{j(x_1)j(x_3)}\right.\right. \\ &\qquad\left.\left. + W_{j(x_3)}W_{j(x_1)j(x_2)}\right) + W_{j(x_1)}W_{j(x_2)}W_{j(x_3)}\right\}Z[j] \\ &= G_{\rm c}^{(3)}(x_1,x_2,x_3) + \left[G_{\rm c}^{(1)}(x_1)G_{\rm c}^{(2)}(x_2,x_3) + 2\text{ perm}\right] + G_{\rm c}^{(1)}(x_1)G_{\rm c}^{(1)}(x_2)G_{\rm c}^{(1)}(x_3). \end{aligned} \tag{12.23}$$

and for the four-point function

$$\begin{aligned} G^{(4)}(x_1,\ldots,x_4) &= G_{\rm c}^{(4)}(x_1,\ldots,x_4) + \left[G_{\rm c}^{(3)}(x_1,x_2,x_3)\,G_{\rm c}^{(1)}(x_4) + 3 \text{ perm}\right] \\ &\quad + \left[G_{\rm c}^{(2)}(x_1,x_2)\,G_{\rm c}^{(2)}(x_3,x_4) + 2 \text{ perm}\right] \\ &\quad + \left[G_{\rm c}^{(2)}(x_1,x_2)\,G_{\rm c}^{(1)}(x_3)\,G_{\rm c}^{(1)}(x_4) + 4 \text{ perm}\right] \\ &\quad + G_{\rm c}^{(1)}(x_1)\cdots G_{\rm c}^{(1)}(x_4). \end{aligned} \tag{12.24}$$

In the pure φ^4-theory (and in normal systems) there are no odd Green functions and we remain with (8.63), which was observed there diagrammatically up to second order in the perturbation expansion.

For the general Green function $G^{(n)}$, the total number of terms is most easily retrieved by dropping all indices and factors i and differentiating with respect to j (the prime stands for $\delta/\delta j$)

$$\begin{aligned} G^{(1)} &= e^{-W}\left(e^{W}\right)_j = W_j = G_{\rm c}^{(1)} \\ G^{(2)} &= e^{-W}\left(e^{W}\right)_j = W_{jj} + W_j^2 = G_{\rm c}^{(2)} + G_{\rm c}^{(1)2} \\ G^{(3)} &= e^{-W}\left(e^{W}\right)_{jjj} = W_{jjj} + 3W_{jj}W_j + W_j^3 = G^{(3)} + 3G_{\rm c}^{(2)}G_{\rm c}^{(1)} + G_{\rm c}^{(1)3} \\ G^{(4)} &= e^{-W}\left(e^{W}\right)_{jjjj} = W_{jjjj} + 4W_{jjj}W_j + 3W_{jj}^2 + 6W_{jj}W_j^2 + W_j^4 \\ &\qquad = G_{\rm c}^{(4)} + 4G_{\rm c}^{(3)}G_{\rm c}^{(1)} + 3G_{\rm c}^{(2)2} + 6G_{\rm c}^{(2)}G_{\rm c}^{(1)2} + G_{\rm c}^{(1)4}. \end{aligned} \tag{12.25}$$

All relations follow from the recursion relation

$$G^{(n)} = G_j^{(n-1)} + G^{(n-1)}G_{\rm c}^{(1)}, \qquad n > 2, \tag{12.26}$$

if one uses $G_{{\rm c}j}^{(n-1)} = G_{\rm c}^{(n)}$ and the initial relation $G^{(1)} = G_{\rm c}^{(1)}$. By comparing the first four relations with the explicit forms (12.22) (12.24) we see that the numerical factors on the right-hand side of (12.25) refer to the permutations of the arguments $x_1, x_2, x_3, \ldots$ of otherwise equal expressions. Since there is no problem in reconstructing the explicit permutations we shall, from now on, write all composition laws in the short-hand notation (12.25).

The formula (12.25) and its generalization is often referred to as *cluster decomposition* or also as the *cumulant expansion* of the Green functions.

Let us now prove the statement that the connected Green functions collect precisely all connected diagrams in the n-point functions. For this we observe that the decomposition rules can be inverted by simply writing $iW[j] = \log Z[j]$ and differentiating such that one finds

$$\begin{aligned} G_{\rm c}^{(1)} &= G^{(1)} \\ G_{\rm c}^{(2)} &= G^{(2)} - G^{(1)}G^{(1)} \\ G_{\rm c}^{(3)} &= G^{(3)} - 3G^{(2)}G^{(1)} + 2G^{(1)3} \\ G_{\rm c}^{(4)} &= G^{(4)} - 4G^{(3)}G^{(1)} + 12G^{(2)}G^{(1)2} - 3G^{(2)2} - 6G^{(1)4}. \end{aligned} \tag{12.27}$$

Each equation follows from the previous one by differentiation with respect to j, and replacing the derivatives on the right-hand side according to the rule

$$G_j^{(n)} = G^{(n+1)} - G^{(n)}G^{(1)}. \tag{12.28}$$

Again the numerical factors imply different permutations of the arguments, and the primes denote functional differentiations with respect to j.

Now it is obvious that any connected diagram contained in $G^{(n)}$ must also be contained in $G_{\rm c}^{(n)}$, since all the terms added or subtracted in (12.27) are products of $G^{(n)}$'s and thus necessarily disconnected.

The proof that $G_{\rm c}^{(n)}$ collects *only* connected diagrams, is somewhat more involved and requires the use of the equations of motion (12.8). Since the information on $G_{\rm c}$ is contained most directly in $W[j]$, we shall first translate these equations into a functional differential equation for $W[j]$.

12.4 Functional Differential Equation for $W[j]$

Since we already know the consequences of the equation of motion for $Z[j]$ we may simply insert (12.17) into (12.16) and find directly the following differential equation for $W[j]$:

$$iG_0^{-1}W_j - \frac{1}{2!}V_3\frac{1}{i^2}\left(iW_{jj} - W_j^2\right) - \frac{1}{3!}V_4\frac{1}{i^3}\left(iW_{jjj} - 3W_{jj}W_j - iW_j^3\right) + j = 0. \tag{12.29}$$

Multiplying this by $-iG_0$ gives

$$W_j = -iG_0\frac{1}{2!}V_3\frac{1}{i^2}\left(iW_{jj} - W_j^2\right) - iG_0\frac{1}{3!}V_4\frac{1}{i^3}\left(iW_{jjj} - 3W_{jj}W_j - iW_j^3\right) + iG_0 j. \tag{12.30}$$

This may be expressed in terms of the connected j-Green function

$$G_{\rm c}^{(1)} = W_j(x) \tag{12.31}$$

as

$$\begin{aligned} G_{\rm c}^{(1)} &= -G_0\frac{V_3}{2!}\left(G_{{\rm c}j}^{(1)} + iG_{\rm c}^{(1)}G_{\rm c}^{(1)}\right) \\ &\quad +G_0\frac{V_4}{3!}\left(iG_{{\rm c}jj}^{(1)} - 3G_{{\rm c}j}^{(1)}G_{\rm c}^{(1)} - iG_{\rm c}^{(1)3}\right) + iG_0 j. \end{aligned} \tag{12.32}$$

12.5 Iterative Solution

Equation (12.30) can best be solved graphically as shown in Fig. 12.1. The lowest,

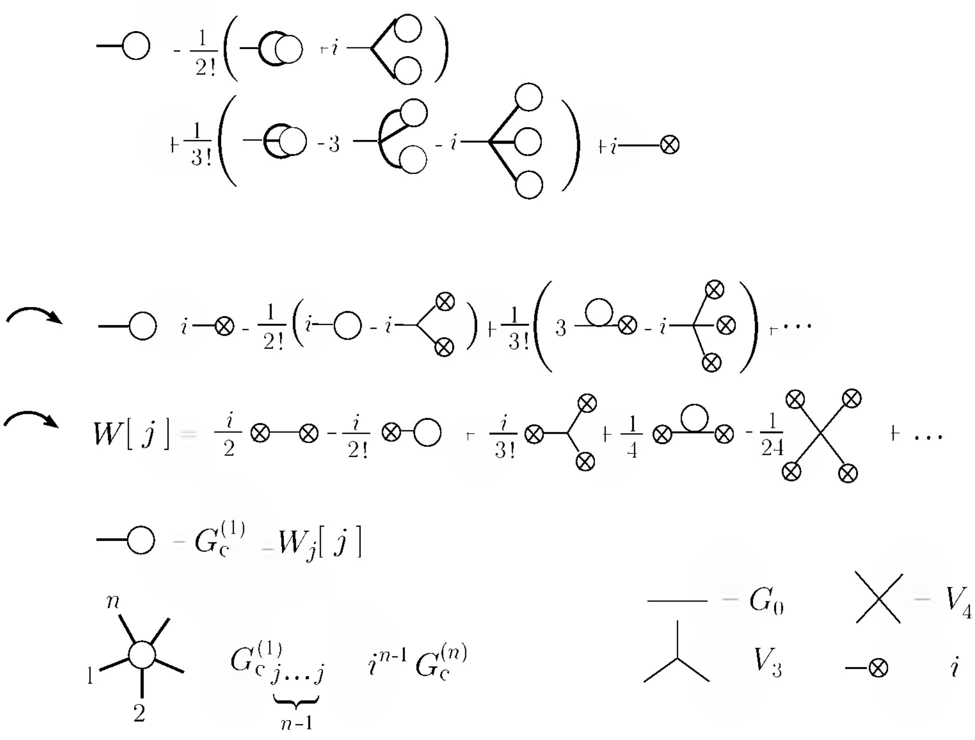

$-\frac{1}{2!}$
$+i$
$+\frac{1}{3!}$
-3
$-i$
$+i$
i
$-\frac{1}{2!}$
$-i$
$+\frac{1}{3!}$
3
$-i$
$+\cdots$
$W[j]=\frac{i}{2}$
$-\frac{i}{2!}$
$+\frac{i}{3!}$
$+\frac{1}{4}$
$-\frac{1}{24}$
$+\ldots$
$=G_c^{(1)}=W_j[j]$
n
1
2
$G_c^{(1)}{}_{\underbrace{j\ldots j}_{n-1}}$
$i^{n-1}G_c^{(n)}$
$=G_0$
$=V_4$
V_3
i

FIGURE 12.1 Graphical solution of recursion relation (12.30) for the generating functional $W[j]$ of all connected Green functions.

zeroth order in V_3, V_4, we have[1]

$$G_c^{(1)} = iG_0\, j. \tag{12.33}$$

From this we find the zeroth order generating functional $W[j]$ by functional integration

$$W^0[j] \;=\; \int \mathcal{D}j\, W_j^{(0)}[j] = \int \mathcal{D}_j G_c^{(1)} = \frac{i}{2} jG_0 j, \tag{12.34}$$

a result already known from previous discussions.

Reinserting (12.34) on the right-hand side of (12.32) we find the first-order equation

$$G_c^{(1)} \;=\; -G_0\frac{V_3}{2!}\left(iG_0 - iG_0 j\, G_0 j\right) + G_0\frac{V_4}{3!}\left[3G_0G_0 j - (G_0 j)^3\right] + iG_0 j. \tag{12.35}$$

---

[1] The superscripts (1), (2), ... on Green functions $G_c^{(1)}$, $G_c^{(2)}, \ldots$ refer to the number of points in the connected Green function, while those on W^1, $W^2, \ldots$ record the order in the interactions $V_{3,4}$ of the perturbative expressions.

This can be integrated functionally to obtain $W[j]$ up to first order in the potentials. Graphically, this process amounts to multiplying the open line in each diagram by a current j and dividing the resulting powers j^n by n. Thus we have (see Fig. 12.1)

$$\begin{aligned} W^0[j] + W^1[j] &= \frac{i}{2} j G_0 j - \frac{i}{2!} j G_0 V_3 G_0 + \frac{i}{3!} V_3 \left(G_0 j\right)^3 \\ &+ \frac{1}{4} V_4 G_0 \left(G_0 j\right)^2 - \frac{1}{24} V_4 \left(G_0 j\right)^4 . \end{aligned} \qquad (12.36)$$

This procedure can be continued to any order in V_3, V_4.

We are now in a position to confirm the statement made above that the generating functional $W[j]$ collects *only* connected diagrams in its Taylor coefficients $\delta^n W/\delta j(x_1) \dots \delta j(x_n)$. Recall that we convinced ourselves by the argument after Eq. (12.28) that these were *all* connected diagrams contained in $G^{(n)}(x_1, \dots, x_n)$. For the lowest two orders we can verify the connectedness directly by inspecting the third line in Fig. 12.1. After this, the diagrammatic form of the recursion relation shows that this topological property remains true to all orders in $V_{3,4}$, by induction. Since, if it was true for some n, then all $G_c^{(1)}$ to be inserted on the right-hand side are connected and so are the diagrams constructed from these giving $G_c^{(1)}$ to $(n+1)$st order. Note that this calculation is unable to recover the value of $W[j]$ at $j = 0$ since this is an unknown integration constant of the functional differential equation. For the purpose of generating Green functions, this constant is irrelevant. We have seen in Eq. (8.68) that $Z[0]$ consists of the sum of all connected vacuum diagrams contained in $W[0]$.

12.6 Vertex Functions

Having understood the connectedness structure of Feynman diagrams, we now turn to the second important composition property: that in terms of one-particle irreducible graphs. A crucial role in the perturbation expansions of Chapter 8 was played by the vertex functions [the one-particle irreducible amputated Green functions introduced on p. 475]. In his section we shall describe their properties by functional differential equations. In particular, we shall present a simple algorithm yielding the composition rules of connected diagrams into one-particle irreducible ones.

12.7 The Generating Functional for Vertex Functions

First we introduce a new generating functional $\Gamma[\Phi]$ which is defined as the Legendre transform of $W[j]$:

$$\Gamma[\Phi] \equiv W[j] - W_j\, j, \qquad (12.37)$$

where $W_j\, j$ is a short-hand notation for

$$W_j\, j = \int d^D x\, W_j(x)\, j(x), \qquad (12.38)$$

and the new variable Φ is the functional derivative of $W[j]$:

$$\Phi(x) \equiv \frac{\delta W[j]}{\delta j(x)} \equiv W_j = \langle\varphi\rangle_j, \tag{12.39}$$

thus giving the ground state expectation of the field operator in the presence of the current j. The physical situation corresponds to $j = 0$ and we shall denote the associated field expectation by

$$\Phi_0 = \langle\varphi\rangle|_{j=0}, \tag{12.40}$$

which may be zero or non-zero and space-time dependent. The most common situation found in quantum field theoretic systems is $\Phi_0 = 0$. In many interesting physical applications to many-body systems, however, the state Φ_0 at $j = 0$ is non-zero and in fact, not even isotropic, but carries interesting structures: It may be perforated by vortices, as in superconductors, exhibit a plane wave-like modulation, as in magnetic superconductors and pion condensates, or occur in a lattice-like modulation, as in the blue phase of cholesteric liquid crystals. At present we shall allow for any such possibility.

In this section we want to demonstrate an important property of the functional derivatives of $\Gamma[\Phi]$

$$\Gamma^{(n)}_{\Phi\ldots\Phi}(x_1, \ldots, x_n) \equiv \frac{\delta}{\delta\Phi(x_1)} \cdots \frac{\delta}{\delta\Phi(x_n)}\Gamma[\Phi]\,. \tag{12.41}$$

They collect precisely all OPI vertex diagrams formed with vertices $V_3 + V_4\Phi$ and V_4, and with propagators $G_0 \equiv \mathcal{A}^{-1}_{\Phi\Phi}|$. The expression $V_4\Phi$ is short notation for $\int d^D x V_4(x_1, x_2, x_3, x_4)\Phi(x_4)$. With the above Thus in the previously discussed special case of a φ^4-theory with $\Phi_0 = \langle\varphi\rangle = 0$, the vertex functions (12.41) for $\Phi = 0$ coincide with those defined graphically in Eq. (8.6.1), for example.

In order to prove this, we take again recourse to a functional differential equation for $\Gamma[\Phi]$. This can be derived quite simply from that for $W[j]$. First we observe that $G^{(1)}_{\rm c}$ is simply the field expectation Φ. Second we see that

$$iG^{(2)}_{\rm c} = G^{(1)}_j = W_{jj} = \frac{\delta\Phi}{\delta j} = \left(\frac{\delta j}{\delta\Phi}\right)^{-1} = -\Gamma^{-1}_{\Phi\Phi}. \tag{12.42}$$

Here the inverse is to be understood in the functional sense, i.e.,

$$\Gamma^{-1}_{\Phi\Phi}(x, y) \equiv \left[\frac{\delta^2\Gamma}{\delta\Phi(x)\delta\Phi(y)}\right]^{-1} \tag{12.43}$$

is the functional matrix which satisfies

$$\int dy\, \Gamma^{-1}_{\Phi\Phi}(x, y)\Gamma_{\Phi\Phi}(y, z) = \delta(x - z). \tag{12.44}$$

Equation (12.42) says that the second derivative of the generating functional $\Gamma[\Phi]$ determines directly the propagator of the interacting theory in the presence of the external source j. Since j is an auxiliary quantity which eventually has to be turned off such that Φ becomes Φ_0, the actual physical propagator is given by

$$G = G_{\rm c}^{(2)} = i\Gamma_{\Phi\Phi}^{-1} \,, \tag{12.45}$$

evaluated at $\Phi = \Phi_0$. The third relation to be used follows from (12.42) by applying the chain rule and deriving once more functionally with respect to j.

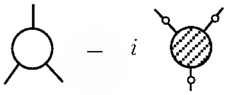
$$W_{jjj} = \Gamma_{\Phi\Phi}^{-2}\Gamma_{\Phi\Phi\Phi}\frac{\delta\Phi}{\delta j} = -\Gamma_{\Phi\Phi}^{-3}\Gamma_{\Phi\Phi\Phi} = -iG^3\Gamma_{\Phi\Phi\Phi}. \tag{12.46}$$

This equation has a simple physical meaning. The third derivative of $W[j]$ on the left-hand side is the full three-point function (up to the sign), so that

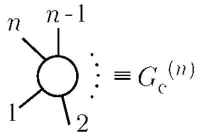
$$G^{(3)} = -W_{jjj} = iG^3\Gamma_{\Phi\Phi\Phi}. \tag{12.47}$$

This equation states that the full three-point function arises from a third derivative of $\Gamma[\Phi]$ by attaching to each derivation a full propagator. This is exactly the structure observed before in (8.72) for the four-point function.

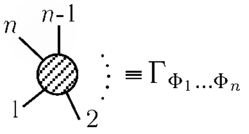
We shall express Eq. (12.52) graphically as follows:



where



denotes the connected n-point function and



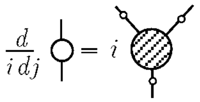
the n-point vertex function.

Thus $\Gamma_{\Phi\Phi\Phi}$ seems to be a three-point vertex function in the same sense as defined graphically in Subsection 8.6.1. For this it has to contain all OPI diagrams. This will emerge from the discussion to follow.

To go on to higher orders, we observe that (12.46) states that the functional derivative of the full propagator G with respect to the current j is

$$\frac{1}{i}G_j = -W_{jjj} = G^{(3)} = iG^3\Gamma_{\Phi\Phi\Phi}. \tag{12.48}$$

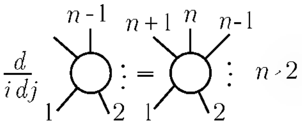
This is pictured graphically as follows:



This equation may be differentiated further with respect to the current j by graphical methods. From the definition (12.18) we deduce the trivial recursion relation

$$G_{\rm c}^{(n)}\left(x_1,\ldots,x_n\right)=\frac{\delta}{i\delta j(x_1)}G_{\rm c}^{(n-1)}\left(x_2,\ldots,x_n\right), \tag{12.49}$$

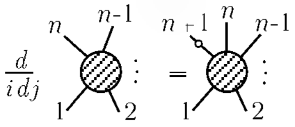
which is represented graphically as



Thus, by applying $\delta/i\delta j$ repeatedly to Eq. (12.48), we generate all higher connected Green functions. On the right-hand side of (12.48), the differentiation of each line is done using once more (12.48), which changes a line into a three-point function. It remains to find the derivative of the vertex function. This is calculated via the chain rule as

$$\Gamma_{\Phi\ldots\Phi j}=\Gamma_{\Phi\ldots\Phi\Phi}\frac{\delta\Phi}{\delta j}=\Gamma_{\Phi\ldots\Phi\Phi}iG, \tag{12.50}$$

which is represented graphically as



With these graphical rules, we can differentiate (12.46) any number of times, and derive the graphical structure of the connected Green functions with an arbitrary number of external legs. The result up to $n=5$ is shown in Fig. 12.2.

The diagrams generated in this way have a tree-like structure which is why they are called *tree diagrams*. The tree decomposition reduces all diagrams to their one-particle irreducible contents.

The one-particle reducible structure of all graphs can also be illustrated in another way. Let us separate the effective action into a free and a nontrivial part

$$\begin{aligned}\Gamma[\Phi] &\equiv \Gamma^0[\Phi]+\Gamma^{\rm int}[\Phi]=\frac{1}{2}\left(\partial\Phi\right)^2-\frac{m^2}{2}\Phi^2+\Gamma^{\rm int}[\Phi]\\ &= \frac{1}{2}\Phi iG_0^{-1}\Phi+\Gamma^{\rm int}[\Phi].\end{aligned} \tag{12.51}$$

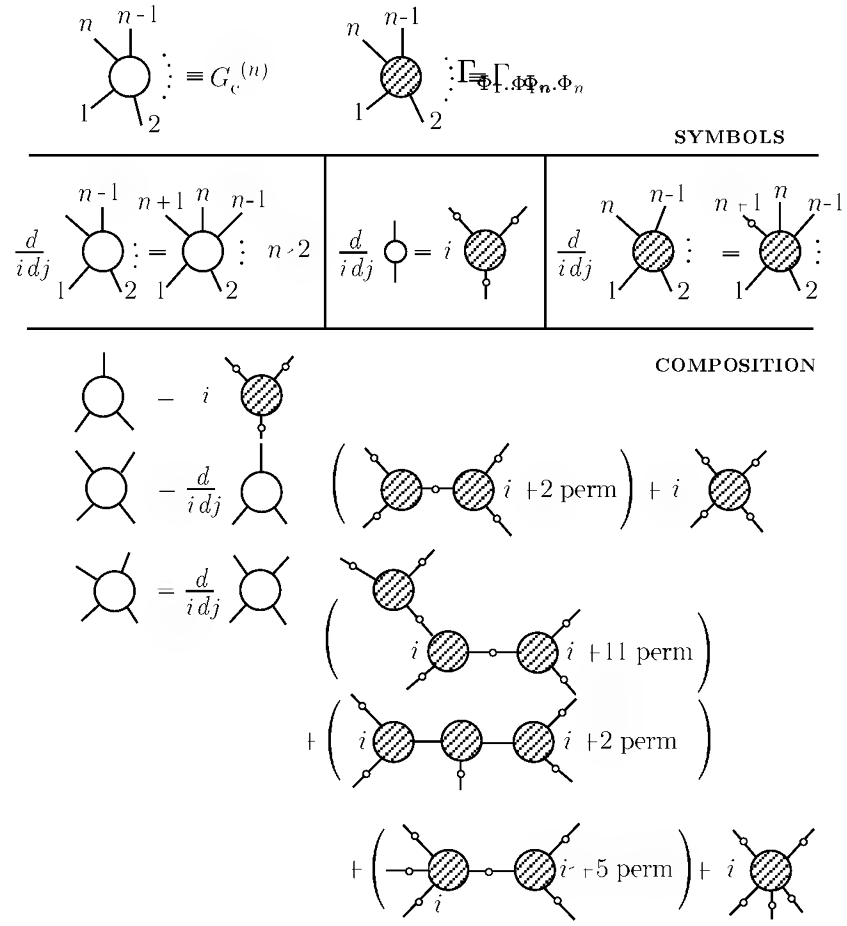


FIGURE 12.2 Tree decompositon of connected Green functions into one-particle irreducible perts.

The free part coincides with the free action $\mathcal{A}^0[\Phi]$ in Eq. (12.2), except that the fluctuating field φ is replaced by its expectation value Φ. The same decomposition is done with the generating functional $W[j]$ [recall (12.34)]:

$$W[j] \;=\; W^0[j]+W^{\rm int}[j]=\frac{i}{2}j\,G_0\,j+W^{\rm int}[j]. \tag{12.52}$$

Then we see that

$$\begin{aligned}\Gamma^{\rm int}[\Phi] \;&=\; W^{\rm int}[j]-\frac{i}{2}\Phi G_0^{-1}\Phi\\ &\quad+\frac{i}{2}jG_0j-j\Phi.\end{aligned} \tag{12.53}$$

But using the equation for the current

$$j=-\Gamma_\Phi=-\Gamma_\Phi^{\rm int}-iG_0^{-1}\Phi \tag{12.54}$$

we find

$$\frac{i}{2}\Gamma_{\Phi}^{\rm int}G_0\Gamma_{\Phi}^{\rm int}=\frac{i}{2}jG_0j-\frac{i}{2}\Phi G_0^{-1}\Phi-j\Phi \tag{12.55}$$

which is obviously a one-particle reducible contribution. Inserting this into (12.53), we may write

$$W^{\rm int}[j]=\Gamma^{\rm int}[\Phi]-\frac{i}{2}\Gamma_{\Phi}^{\rm int}G_0\Gamma_{\Phi}^{\rm int}. \tag{12.56}$$

This equation shows explicitly how the sum of all connected diagrams in $W^{\rm int}[j]$ is composed of all particle irreducible connected diagrams in $\Gamma^{\rm int}[\Phi]$ plus all one-particle *reducible* diagrams.

The effective action $\Gamma[\Phi]$ can also be used to prove the fact that the full propagator can be expressed as a geometric series (8.71) of repetitions of the self-energy, a fact that was observed graphically to low orders in Subsection 8.6.1. We use once more the decomposition (12.51):

$$\Gamma[\Phi]=\Gamma^0[\Phi]+\Gamma^{\rm int}[\Phi]. \tag{12.57}$$

Differentiating this twice with respect to Φ, we obtain

$$\begin{aligned}\Gamma_{\Phi\Phi} &= iG_0^{-1}+\Gamma_{\Phi\Phi}^{\rm int},\\ \Gamma_{\Phi\Phi\Phi} &= \Gamma_{\Phi\Phi\Phi}^{\rm int},\end{aligned} \tag{12.58}$$

and (12.45) can be rewritten as

$$G=G_0\left(1-iG_0\Gamma_{\Phi\Phi}^{\rm int}\right)^{-1}. \tag{12.59}$$

Expanding the denominator and recollecting terms this can also be written as an integral equation

$$G=G_0+iG_0\Gamma_{\Phi\Phi}^{\rm int}G. \tag{12.60}$$

In this equation we recognize the self-energy

$$\Sigma=-\Gamma_{\Phi\Phi}^{\rm int}. \tag{12.61}$$

This was introduced graphically in Eq. (8.71), where it was *defined* by the relation

$$G\equiv i[iG_0^{-1}-\Sigma]^{-1},\quad \Sigma\equiv iG_0^{-1}-iG^{-1}. \tag{12.62}$$

Comparison with (12.59) shows that (12.61) is the correct identification.

Thus the self-energy is given by the interacting part of the second derivative of the effective action. This proves the statement that, in general, all Feynman diagrams in the propagator can be obtained by a geometric series type of repetition of self-energy diagrams. What we do not know as yet, but what will become clear immediately in the next section is that the self-energy collects precisely all one-particle irreducible amputated two-point functions.

12.8 Functional Differential Equation for $\Gamma[\Phi]$

We shall now prove the fact that $\Gamma[\Phi]$ contains only one-particle irreducible diagrams by means of a functional differential equation for $\Gamma[\Phi]$. For a cubic and quartic interaction, this is immediately obtained from the differential equation (12.29) for $W[j]$. We simply substitute

$$W_j \to \Phi, \quad j \to \Gamma_\Phi, \quad W_{jj} \to iG, \quad W_{jjj} \to -G^{(3)} = -iG^3\Gamma_{\Phi\Phi\Phi}, \tag{12.63}$$

make use of the separation (12.57), and find for the interacting part the functional differential equation

$$\Phi\Gamma^{\rm int}_\Phi = -\frac{1}{2!}V_3\Phi^3 - \frac{1}{3!}V_4\Phi^4 - \frac{1}{2!}\Phi\left(V_3 + V_4\Phi\right)G - \frac{1}{3!}\Phi V_4 iG^3\Gamma^{\rm int}_{\Phi\Phi\Phi}. \tag{12.64}$$

This equation can be solved solved iteratively together with (12.59). Before starting it is useful to observe that there exists a trivial relation between $\Gamma[\Phi]$ and $\Phi\Gamma^{\rm int}_\Phi$ which merely consists in a factor $1/n$ in front of every power Φ^n. Thus the diagrams in $\Gamma[\Phi]$ differ from those in $\Phi\Gamma[\Phi]$ only by numerical prefactors. The resulting equations are displayed graphically in Fig. 12.3. First we neglect $\Gamma^{\rm int}$ on the right-hand side of the equation and find the first-order correction $\Gamma^1[\Phi]$ to the interacting part $\Gamma^{\rm int}[\Phi]$:

$$\Gamma^1[\Phi] \;=\; -\frac{1}{3!}V_3\Phi^3 - \frac{1}{4!}V_4\Phi^4 - \frac{1}{2}V_3G_0\Phi - \frac{1}{4}V_4G_0\Phi^2. \tag{12.65}$$

The first two terms are simply the interacting parts of the original action $\mathcal{A}^{\rm int}[\Phi]$ (12.3) with φ replaced by Φ. The remaining two terms are new. They may be obtained by partial contractions in the interacting part of the original interaction (12.3),and setting $\varphi = \Phi$ in the remaining uncontracted fields:

$$\begin{aligned} -\frac{1}{3!}V_3\varphi^3 &\;\to\; -\frac{1}{3!}V_3\,3\,\dot\varphi\dot\varphi\,\Phi, \\ -\frac{1}{4!}V_4\varphi^4 &\;\to\; -\frac{1}{4!}V_4\frac{4\cdot 3}{2!}\dot\varphi\dot\varphi\,\Phi\Phi. \end{aligned} \tag{12.66}$$

The iteration has been continued graphically up to the second order in the interactions in Fig. 12.3.

The lowest term $\Gamma^1[\Phi]$ contains obviously only OPI diagrams. The graphical iteration shows that this property persists to all orders. If all diagrams of nth order are OPI, those composed to next order on the right-hand side of Eq. (12.64) always contain at least two more lines and thus do not decompose by cutting a single line. They are therefore are OPI (in normal field theories in which the expectation Φ_0 vanishes at zero external source j). This proves the statement made on that behalf in the beginning. It is thereby confirmed that the selfenergy collects only one-particle irreducible vertex diagrams. Thus the full propagator is indeed obtained from the geometric iteration of such diagrams implied by (12.59):

$$G \;=\; G_0 + G_0(-i\Sigma)G_0 + G_0(-i\Sigma)G_0(-i\Sigma)G_0 + \ldots\;. \tag{12.67}$$

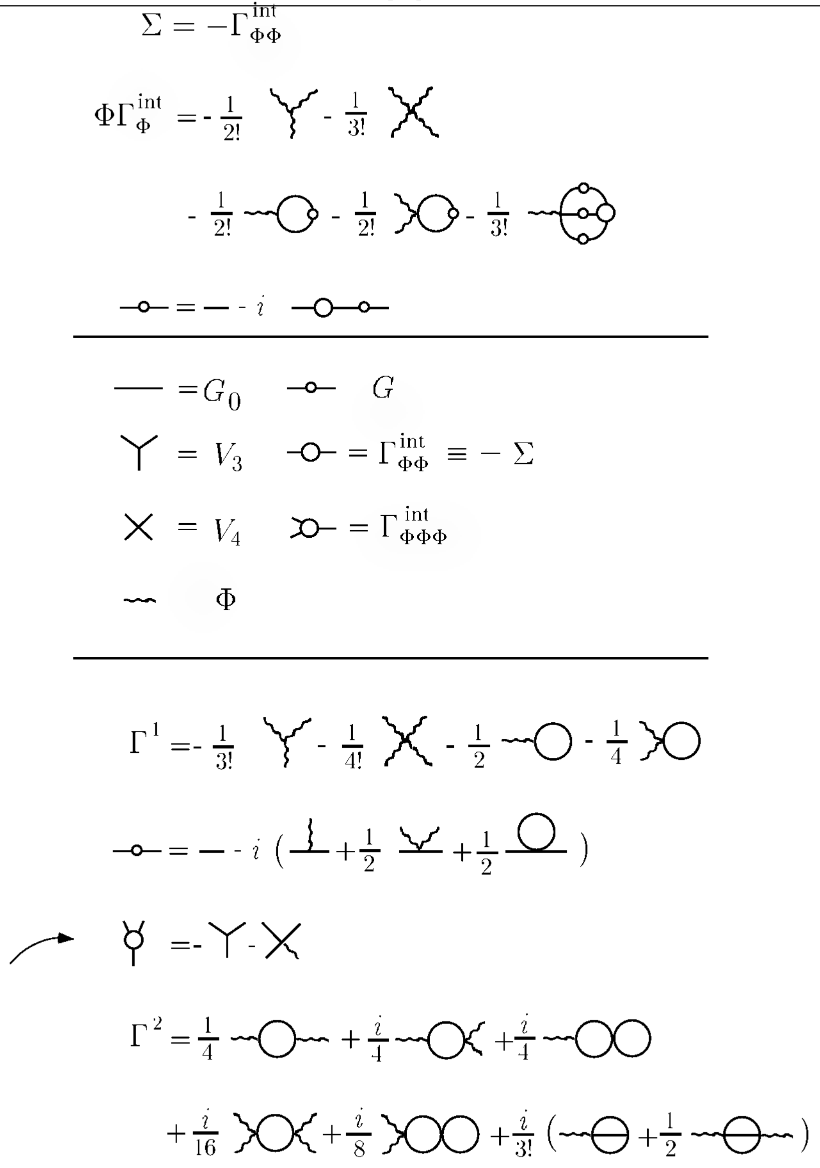

Σ = −Γ int ΦΦ
ΦΓ int Φ = - 1/2! - 1/3!
- 1/2! - 1/2! - 1/3!
= — - i
= G0
G
= V3
= Γ int ΦΦ ≡ − Σ
= V4
= Γ int ΦΦΦ
Φ
Γ1 =- 1/3! - 1/4! - 1/2 - 1/4
= — - i (+ 1/2 + 1/2)
=- -
Γ2 = 1/4 + i/4 + i/4
+ i/16 + i/8 + i/3! (+ 1/2)

FIGURE 12.3 Graphical solution of functional differential equation (12.64) for the interacting part $\Gamma^{\rm int}[\Phi]$ of the effective action.

As argued before, all OPI two-point vertex diagrams must be contained in $\Sigma = -i\Gamma^{\rm int}_{\Phi\Phi}$ since if it occurs in G it must also occur in Σ.

We have also proved the another important statement observed graphically in the low-order diagrams of Chapter 8. All n-point functions can be obtained by composing all OPI vertex diagrams and full Green functions will be via tree diagrams. The composition rules were derived above.

For completeness, let us treat the functional differential equation for $\Gamma[\Phi]$ once more in a different way in a non-normal system (corresponding to a magnetized phase in solid-state physics) with a nonvanishing field expectation $\Phi_0 = \langle\varphi\rangle \neq 0$ for e $j = 0$, keeping explicit reference to Φ_0. Setting

$$\Phi = \Phi_0 + \Phi' \tag{12.68}$$

we define

$$\Gamma'[\Phi'] \equiv \Gamma\left[\Phi_0 + \Phi'\right] \tag{12.69}$$

which then satisfies the equation

$$\begin{aligned} &iG_0^{-1}\Phi_0 - \frac{1}{2!}V_3\left(\Phi_0' + 2\Phi_0\Phi'\right) - \frac{1}{3!}V_4\left(\Phi_0^3 + 3\Phi_0^2\Phi' + 3\Phi_0\Phi'\right) \\ &\quad -\frac{1}{2}V_4 i{\Gamma'}_{\Phi\Phi'}^{-1}\Phi_0 - \frac{1}{2!}V_3\left(i{\Gamma'}_{\Phi\Phi}^{-1} + \Phi'^2\right) \\ &\quad -\frac{1}{4!}V_4\left(\Gamma'^{-3}_{\Phi\Phi}\Gamma_{\Phi'\Phi'\Phi'} + 3i\Gamma_{\Phi'\Phi'}^{-1}\Phi' + \Phi'^3 + 2\Phi_0^2\Phi'^2\right) - \Gamma'_{\Phi'} = 0. \end{aligned} \tag{12.70}$$

Let us now split

$$\Gamma'[\Phi'] = \Gamma'^0[\Phi'] + \Gamma'^{\rm int}[\Phi'], \tag{12.71}$$

with

$$\Gamma^0[\Phi'] \;=\; \mathcal{A}[\Phi_0] + \mathcal{A}_\Phi[\Phi_0]\Phi' + \frac{1}{2}\mathcal{A}_{\Phi\Phi}[\Phi_0]\Phi'\Phi'. \tag{12.72}$$

Inserting this into (12.70), we find for Γ' the functional differential equation

$$\begin{aligned} \Phi'\Gamma'_{\Phi'} \;=\; &-\frac{1}{2!}\Phi'\left(V_3 + V_4\Phi_0\right)\left(i{\Gamma'}_{\Phi'\Phi'}^{-1} + \Phi'^2\right) \\ &-\frac{1}{3!}\Phi' V_4\left({\Gamma'}_{\Phi'\Phi'}^{-3}\Gamma_{\Phi'\Phi'\Phi'} + 3i\Gamma_{\Phi\Phi'}^{-1}\Phi' + \Phi'^3\right). \end{aligned} \tag{12.73}$$

Here we insert

$$\Gamma'_{\Phi\Phi'} = \mathcal{A}_{\Phi\Phi}[\Phi_0] + \Gamma'^{\rm int}_{\Phi'\Phi'} \tag{12.74}$$

and

$$\Gamma'_{\Phi'\Phi'\Phi'} = \Gamma'^{\rm int}_{\Phi'\Phi'\Phi'}. \tag{12.75}$$

Then Eq. (12.73) becomes structurally identical with (12.64), only that V_3, V_4 are replaced by $(V_3 + V_4\Phi_0)$ and V_4, respectively, and the free Green function G_0 by

$${G_0}^{\Phi_0} = i\left[iG_0^{-1} - V_3\Phi_0 - \frac{V_4}{2}\Phi_0^2\right]. \tag{12.76}$$

Thus $\Gamma^{\rm int}[\Phi]$, when expanded in powers of Φ', does indeed collect only one-particle irreducible diagrams. This is what we wanted to prove in the general case $\Phi_0 \neq 0$ [see (12.41)]:

$$\Gamma^{(n)}_{\Phi'\dots\Phi'} = \left.\frac{\delta^n\Gamma}{\delta\Phi(x)\cdots\delta\Phi(x_n)}\right|_{\Phi=\Phi_0}. \tag{12.77}$$

12.9 Effective Action as a Basis for Variational Calculation

In the last section we have seen that the effective action contains all the information necessary to construct all n point functions. Moreover, its calculation requires only a certain restricted class of Feynman diagrams, namely those which are OPI. There is, however, another important feature which makes the effective action a powerful tool in the study of physical properties of a system and which, finally, justifies its name: Any physical configuration of the field expectation $\Phi = \langle\varphi\rangle|_j$ extremizes $\Gamma[\Phi]$. This is a direct consequence of the definition (12.37). If we write $\Gamma[\Phi]$ in the form

$$\Gamma[\Phi] = W[j] - \int d^D x\, \Phi(x) j(x) \tag{12.78}$$

we find

$$\begin{aligned}\frac{\delta\Gamma}{\delta\Phi} &= \int d^D x \frac{\delta W}{\delta j}\frac{\delta j}{\delta\Phi} \\ &\quad - \int d^D x\, \Phi \frac{\delta j}{\delta\Phi} - j(x) = -j(x).\end{aligned} \tag{12.79}$$

In the absence of the auxiliary external source j, $\Gamma[\Phi]$ is indeed extremal. Thus, the functional $\Gamma[\Phi]$ has exactly the same property in quantum theory as the usual action $\mathcal{A}[\Phi]$ in classical theory.

12.10 Effective Potential

A special role in the extraction of observational consequences from a theory will be played by the effective potential. Remember that in classical mechanics, the potential is defined by the action evaluated for a time-independent orbit $q(t)$ as

$$\mathcal{A} = \int_{t_a}^{t_b} dt \mathcal{L}(q,\dot q)\bigg|_{q=\text{const}} = -TV(q), \qquad T \equiv t_b - t_a. \tag{12.80}$$

In analogy, we define the effective potential of a field theory, if it has the special property $\Phi_0 = \text{const}$, by

$$\Gamma[\Phi]|_{\Phi=\text{const}} = -TL^3 V(\Phi), \qquad L^3 = \text{spatial volume}. \tag{12.81}$$

Comparing this with (12.41) we see that the effective potential has the expansion

$$TL^3 V(\Phi) = -\sum \frac{1}{n!}\int d^D x_1 \cdots d^D x_n \Gamma^{(n)}(x_1,\dots,x_n)\,(\Phi-\Phi_0)\dots(\Phi-\Phi_0)\,. \tag{12.82}$$

Introducing the Fourier transforms

$$\Gamma^{(n)}(q_1,\dots,q_n) \equiv \int d^D x_1 \cdots d^D x_n e^{i(q_1x_1+\ldots+q_nx_n)}\Gamma^{(n)}(x_1,\dots,x_n), \tag{12.83}$$

and removing the overall δ-function of energy-momentum conservation contained in $\Gamma^{(n)}(q_1,\dots,q_n)$ due to the translational invariance of $\Gamma^{(n)}(x_1,\dots,x_n)$,

$$\Gamma^{(n)}(q_1,\dots,q_n) \equiv (2\pi)^D\delta^{(D)}(q_1+\dots+q_n)\bar{\Gamma}^{(n)}(q_1,\dots,q_n), \tag{12.84}$$

we can write (12.86) as

$$V(\Phi) = -\sum \frac{1}{n!}\bar{\Gamma}^{(n)}(q_1,\dots,q_n)\bigg|_{q_i=0}(\Phi-\Phi_0)\dots(\Phi-\Phi_0). \tag{12.85}$$

The discussion has been given for a single Bose field. For a set of Bose fields φ_a, the index a may be imagined as being included in the spacetime index x. Thus Eq. (12.86) reads more explicitly:

$$V(\Phi_a) = -\sum \frac{1}{n!}\,\bar{\Gamma}^{(n)}(q_1,\dots,q_n)\Big|_{q_i=0}(\Phi-\Phi_0)_{a_1}\dots(\Phi-\Phi_0)_{a_n}\,. \tag{12.86}$$

13

Systematic Graphical Construction of Feynman Diagrams and Their Multiplicities

In Section 12.4 we have calculated the generating functional for the connected Green functions $W[j]$ by solving the functional differential equation (12.29) with respect to j. In addition, $W[j]$ may also be considered as a functional of the free propagator G_0. As such it also obeys functional differential equation which can be turned into a recursion relation. This is solved order by order in the coupling constant to find all connected vacuum diagrams with their proper multiplicities. Let us apply this procedure here to $W[0]$ which contains all connected vaccum diagrams, first for a pure ϕ^4-theory, subsequently to a theory with two scalar fields ϕ and A and an interaction $\phi^2 A$.

After obtaining the connected vacuum diagrams, all Feynman diagrams with external lines are obtained from functional derivatives of the connected vacuum diagrams with respect to the free correlation function.

Finally, the recursive graphical construction will be automatized by computer algebra with the help of a unique matrix notation for the Feynman diagrams. The methods developed in this chaoter have been set up a long time ago,[1] but for a long time they have only been solved only for low orders in the coupling strength, and to all orders only for a rather trivial zero-dimensional quantum field theories, the anharmonic integral. Here we present an extension of this work[2] consisting in an efficient graphical algorithm for solving the functional differential equation for $W[0]$ as a functional of G_0. We shall do this first for a multicomponent scalar ϕ^4-theory, then also for a theory with two scalar fields ϕ and A with an interaction $\phi^2 A$.

In a second step, the connected vacuum diagrams are used to derive all connected diagrams with external lines with the help of functional derivatives of the connected vacuum diagrams with respect to the free correlation function. This operation will represented graphically by cutting lines. Finally, we automatize our construction method by computer algebra with the help of a unique matrix notation for Feynman diagrams.

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[1] H. Kleinert, Fortschr. Phys. *30*, 187 (1982); *30*, 351 (1982).

[2] H. Kleinert, Axel Pelster, B. Kastening, and M. Bachmann, (hep-th/9907168). Algebraic program and its output can be downloaded from http://www.physik.fu-berlin.de/~kleinert/294/programs .

13.1 Generalized Scalar ϕ^4-Theory

The folowing treatment will involve somewhat lengthy equations such that it is useful to introduce a a shoter notation for tha symbols used. For the free proagator $G_0(x_1, x_2)$ we shall employ a functional matrix notation G_{12}. The fully interacting two-point function $G(x_1, x_2)$ will be denoted by $\mathbf{G}_{12}$. The D-dimensional integral $\int d^D x_1$ will simply be written as $\int_1$. We shall further work in euclidean spacetime to avoid factors of i. The scalar field ϕ is allowd to have N components, and the thermal flcutuations are controlled by a euclidean action which plays the role of an energy functional:

$$E[\phi] = \frac{1}{2}\int_{12} G_{12}^{-1}\phi_1\phi_2 + \frac{g}{4!}\int_{1234} V_{1234}\phi_1\phi_2\phi_3\phi_4 \tag{13.1}$$

with some coupling constant g. The functional matrix G_{12}^{-1} is the inverse of the free propagator G_{12}. Both contain, in addition , a Kronecker δ for the N field components, which we suppress. Throughout the manipulations to follow, the functional matrix G_{12} will be considered as a completely general symmetric nonsingular functional matrix, such that G_{12}^{-1} exists. Only at the end shall we specify G_{12}, identifying it with the free propagator, i.e., for the inverse

$$G_{12}^{-1} \to G_{\alpha_1,\alpha_2}^{-1}(x_1, x_2) \;=\; \delta_{\alpha_1,\alpha_2}\left(-\partial_{x_1}^2 + m^2\right)\delta(x_1 - x_2)\,, \tag{13.2}$$

In applications to critical phenomena to be discussed in Chapter 21, the mass m^2 will be proportional to the temperature distance $T - T_c$ from the critical point.

The interaction will likewise be considered as a completely general symmetric function of four arguments, $gV(x_1, x_2, x_3, x_4)$, where g parametrizeds the coupling strength and serves as an expansion parameter. In the short-hand notation, it is a symmetric functional tensor of rank four, and will eventuzally be identified with the true interaction

$$\begin{aligned} V_{1234} &\to V_{\alpha_1,\alpha_2,\alpha_3,\alpha_4}(x_1, x_2, x_3, x_4) \qquad\qquad (13.3)\\ &= \frac{1}{3}\left\{\delta_{\alpha_1,\alpha_2}\delta_{\alpha_3,\alpha_4} + \delta_{\alpha_1,\alpha_3}\delta_{\alpha_2,\alpha_4} + \delta_{\alpha_1,\alpha_4}\delta_{\alpha_2,\alpha_3}\right\}\delta(x_1 - x_2)\delta(x_1 - x_3)\delta(x_1 - x_4)\,. \end{aligned}$$

By using natural units in which the Boltzmann constant k_B times the temperature T equals unity, the partition function is determined as a functional integral over the Boltzmann weight $e^{-E[\phi]}$

$$Z = \int \mathcal{D}\phi\, e^{-E[\phi]} \tag{13.4}$$

and may be evaluated perturbatively as a power series in the coupling constant g. From this we obtain the negative free energy $W = \ln Z$ as an expansion

$$W = \sum_{p=0}^{\infty} \frac{1}{p!}\left(\frac{-g}{4!}\right)^p W^{(p)}\,. \tag{13.5}$$

The coefficients $W^{(p)}$ may be displayed as connected vacuum diagrams constructed from lines and vertices. Each line represents a free correlation function

$$1 \text{——} 2 \; \equiv G_{12}\,, \tag{13.6}$$

whose functional inverse G^{-1} appears in the energy functional (13.1), defined by

$$\int_2 G_{12}\, G^{-1}_{23} = \delta_{13}\,. \tag{13.7}$$

The vertices represent an integral over the interaction

$$\times \;\; \equiv \int_{1234} V_{1234}\,. \tag{13.8}$$

To construct all connected vacuum diagrams contributing to $W^{(p)}$ to each order p in perturbation theory, one connects p vertices with $4p$ legs in all possible ways according to Feynman's rules which follow from Wick's expansion of correlation functions into a sum of all pair contractions. This yields an increasing number of Feynman diagrams, each with a certain multiplicity which follows from combinatorics. In total there are $4!^p p!$ ways of ordering the $4p$ legs of the p vertices. This number is reduced by permutations of the legs and the vertices which leave a vacuum diagram invariant. Denoting the number of self-, double, triple and fourfold connections with S, D, T, F, there are $2!^S, 2!^D, 3!^T, 4!^F$ leg permutations. An additional reduction arises from the number N of identical vertex permutations where the vertices remain attached to the lines emerging from them in the same way as before. The resulting multiplicity of a connected vacuum diagram in the ϕ^4-theory is therefore given by the formula[3]

$$M^{E=0}_{\phi^4} = \frac{4!^p\, p!}{2!^{S+D}\, 3!^T\, 4!^F\, N}\,. \tag{13.9}$$

The superscript E records that the number of external legs of the connected vacuum diagrams is zero. The diagrammatic representation of the coefficients $W^{(p)}$ in the expansion (13.5) of the negative free energy W is displayed in Table 13.1 up to five loops[4]

For higher orders, the factorially increasing number of diagrams makes it more and more difficult to construct all topologically different diagrams and to count their multiplicities. In particular, it becomes quite hard to identify by inspection the number N of identical vertex permutations. This identification problem is solved by introducing a uniqued matrix notation for the graphs, to be explained in detail in Section IV.

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[3] H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4-Theories*, World Scientific, Singapore, 2000.

[4] B. Kastening, Phys. Rev. D *54*, 3965 (1996); Phys. Rev. D *57*, 3567 (1998); S.A. Larin, M. Mönnigmann, M. Strösser, V. Dohm, Phys. Rev. B *58*, 3394 (1998).

In the following, we shall generate iteratively all connected vacuum diagrams. We start in Subsection II.A by identifying graphical operations associated with functional derivatives with respect to the inverse propagator G^{-1}, or the propagator G. In Subsection II.B we show that these operations can be applied to the one-loop contribution of the free partition function to generate all perturbative contributions to the partition function (13.4). In Subsection II.C we derive a nonlinear functional differential equation for the negative free energy W, whose graphical solution in Subsection II.D. yields all connected vacuum diagrams order by order in the coupling strength.

13.2 Basic Graphical Operations

Each Feynman diagram is composed of integrals over products of free correlation functions G and may thus be considered as a functional of the inverse propagator G^{-1}. The connected vacuum diagrams satisfy a certain functional differential equation, from which they will be constructed recursively. This will be done by a graphical procedure, for which we set up the necessary graphical rules in this subsection. First we observe that functional derivatives with respect to the inverse propagator G^{-1} or to the free propagator G correspond to the graphical prescriptions of cutting or of removing a single line of a diagram in all possible ways, respectively.

13.2.1 Cutting Lines

Since ϕ is a real scalar field, the inverse propagator G^{-1} is a symmetric functional matrix. This property has to be taken into account when performing functional derivatives with respect to the inverse propagator G^{-1}, whose basic rule is

$$\frac{\delta G^{-1}_{12}}{\delta G^{-1}_{34}} = \frac{1}{2}\left\{\delta_{13}\delta_{42} + \delta_{14}\delta_{32}\right\} . \tag{13.10}$$

¿From the identity (13.7) and the functional chain rule, we find the effect of this derivative on the free propagator

$$-\,2\,\frac{\delta G_{12}}{\delta G^{-1}_{34}} = G_{13}G_{42} + G_{14}G_{32} \,. \tag{13.11}$$

This has the graphical representation

$$-2\,\frac{\delta}{\delta G^{-1}_{34}}\;\; {\scriptstyle 1}\;\text{——}\;{\scriptstyle 2} \;=\; {\scriptstyle 1}\;\text{——}\;{\scriptstyle 3}\quad {\scriptstyle 4}\;\text{——}\;{\scriptstyle 2} \;+\; {\scriptstyle 1}\;\text{——}\;{\scriptstyle 4}\quad {\scriptstyle 3}\;\text{——}\;{\scriptstyle 2}\;. \tag{13.12}$$

Thus differentiating a propagator with respect to the inverse propagator G^{-1} amounts to cutting the associated line into two pieces. The differentiation rule (13.10) ensures that the spatial indices of the inverse propagator are symmetrically attached to the newly created line ends in the two possible ways. When differentiating a general Feynman integral with respect to G^{-1}, the product rule of functional differentiation leads to a sum of diagrams in which each line is cut once.

With this graphical operation, the product of two fields can be rewritten as a derivative of the energy functional with respect to the inverse propagator

$$\phi_1\phi_2 = 2\,\frac{\delta E[\phi]}{\delta G_{12}^{-1}}\,, \tag{13.13}$$

as follows directly from (13.1) and (13.10). Applying the substitution rule (13.13) to the functional integral for the fully interacting two-point function

$$\mathbf{G}_{12} = \frac{1}{Z}\int \mathcal{D}\phi\,\phi_1\phi_2\,e^{-E[\phi]}\,, \tag{13.14}$$

we obtain the fundamental identity

$$\mathbf{G}_{12} = -2\,\frac{\delta W}{\delta G_{12}^{-1}}\,. \tag{13.15}$$

Thus, by cutting a line of the connected vacuum diagrams in all possible ways, we obtain all diagrams of the fully interacting two-point function. Analytically this has a Taylor series expansion in powers of the coupling constant g similar to (13.5)

$$\mathbf{G}_{12} = \sum_{p=0}^{\infty}\frac{1}{p!}\left(\frac{-g}{4!}\right)^p \mathbf{G}_{12}^{(p)} \tag{13.16}$$

with coefficients

$$\mathbf{G}_{12}^{(p)} = -2\,\frac{\delta W^{(p)}}{\delta G_{12}^{-1}}. \tag{13.17}$$

The cutting prescription (13.15) converts the vacuum diagrams of pth order in the coefficients $W^{(p)}$ in Table 13.1 to the corresponding ones in the coefficients $\mathbf{G}_{12}^{(p)}$ of the two-point function. The results are shown in Table 13.2 up to four loops. The numbering of diagrams used in Table 13.2 reveals from which connected vacuum diagrams they are obtained by cutting a line.

For instance, the diagrams #15.1-#15.5 and their multiplicities in Table 13.2 follow from the connected vacuum diagram #15 in Table 13.1. We observe that the multiplicity of a diagram of a two-point function obeys a formula similar to (13.9):

$$M_{\phi^4}^{E=2} = \frac{4!^p\,p!\,2!}{2!^{S+D}\,3!^T\,N}\,. \tag{13.18}$$

In the numerator, the $4!^p\,p!$ permutations of the $4p$ legs of the p vertices are multiplied by a factor 2! for the permutations of the $E = 2$ end points of the two-point function. The number N in the denominator counts the identical permutations of both the p vertices and the two end points.

Performing a differentiation of the two-point function (13.14) with respect to the inverse propagator G^{-1} yields

$$-2\,\frac{\delta \mathbf{G}_{12}}{\delta G^{-1}_{34}} = \mathbf{G}_{1234} - \mathbf{G}_{12}\mathbf{G}_{34}\,, \tag{13.19}$$

where $\mathbf{G}_{1234}$ denotes the fully interacting four-point function

$$\mathbf{G}_{1234} = \frac{1}{Z}\int \mathcal{D}\phi\,\phi_1\phi_2\phi_3\phi_4\,e^{-E[\phi]}\,. \tag{13.20}$$

The term $\mathbf{G}_{12}\mathbf{G}_{34}$ in (13.19) subtracts a certain set of disconnected diagrams from $\mathbf{G}_{1234}$. By subtracting *all* disconnected diagrams from $\mathbf{G}_{1234}$, we obtain the connected four-point function

$$\mathbf{G}^{\mathrm{c}}_{1234} \equiv \mathbf{G}_{1234} - \mathbf{G}_{12}\mathbf{G}_{34} - \mathbf{G}_{13}\mathbf{G}_{24} - \mathbf{G}_{14}\mathbf{G}_{23} \tag{13.21}$$

in the form

$$\mathbf{G}^{\mathrm{c}}_{1234} = -2\,\frac{\delta \mathbf{G}_{12}}{\delta G^{-1}_{34}} - \mathbf{G}_{13}\mathbf{G}_{24} - \mathbf{G}_{14}\mathbf{G}_{23}\,. \tag{13.22}$$

The first term contains all diagrams obtained by cutting a line in the diagrams of the two-point-function $\mathbf{G}_{12}$. The second and third terms remove from these the disconnected diagrams. In this way we obtain the perturbative expansion

$$\mathbf{G}^{\mathrm{c}}_{1234} = \sum_{p=1}^{\infty}\frac{1}{p!}\left(\frac{-g}{4!}\right)^{p}\mathbf{G}^{\mathrm{c},(p)}_{1234} \tag{13.23}$$

with coefficients

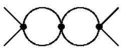
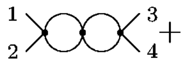
$$\mathbf{G}^{c,(p)}_{1234} = -2\,\frac{\delta \mathbf{G}^{(p)}_{12}}{\delta G^{-1}_{34}} - \sum_{q=0}^{p}\binom{p}{q}\left(\mathbf{G}^{(p-q)}_{13}\mathbf{G}^{(q)}_{24} + \mathbf{G}^{(p-q)}_{14}\mathbf{G}^{(q)}_{23}\right). \tag{13.24}$$

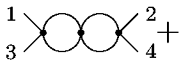
They are listed diagrammatically in Table 13.3 up to three loops. As before in Table II, the multiple numbering in Table 13.3 indicates the origin of each diagram of the connected four-point function. For instance, the diagram #11.2.2, #11.4.3, #14.1.2, #14.3.3 in Table 13.3 stems together with its multiplicity from the diagrams #11.2, #11.4, #14.1, #14.3 in Table 13.2.

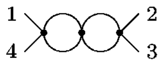
The multiplicity of each diagram of a connected four-point function obeys a formula similar to (13.18):

$$M^{E=4}_{\phi^4} = \frac{4!^p\,p!\,4!}{2!^{S+D}\,3!^T\,N}\,. \tag{13.25}$$

This multiplicity decomposes into equal parts if the spatial indices $1, 2, 3, 4$ are assigned to the $E = 4$ end points of the connected four-point function, for instance:

62208  $\equiv$ 20736 

$+$ 20736 

$+$ 20736 

. (13.26)

Generalizing the multiplicities (13.9), (13.18), and (13.25) for connected vacuum diagrams, two- and four-point functions to an arbitrary connected correlation function with an even number E of end points, we see that

$$M^E_{\phi^4} = \frac{4!^p \, p! \, E!}{2!^{S+D} \, 3!^T \, 4!^F \, N}, \tag{13.27}$$

where N counts the number of permutations of vertices and external lines which leave the diagram unchanged.

13.2.2 Removing Lines

We now study the graphical effect of functional derivatives with respect to the free propagator G, where the basic differentiation rule (13.10) becomes

$$\frac{\delta G_{12}}{\delta G_{34}} = \frac{1}{2} \left\{ \delta_{13} \delta_{42} + \delta_{14} \delta_{32} \right\} . \tag{13.28}$$

We represent this graphically by extending the elements of Feynman diagrams by an open dot with two labeled line ends representing the delta function:

$$1 \!-\!\!\circ\!\!-\! 2 = \quad \delta_{12} \, . \tag{13.29}$$

Thus we can write the differentiation (13.28) graphically as follows:

$$\frac{\delta}{\delta 3 \!-\!\!-\! 4} \; 1 \;\text{——}\; 2 = \frac{1}{2} \left\{ 1 \!-\!\!\circ\!\!-\! 3 \quad 4 \!-\!\!\circ\!\!-\! 2 \quad + \quad 1 \!-\!\!\circ\!\!-\! 4 \quad 3 \!-\!\!\circ\!\!-\! 2 \right\} . \tag{13.30}$$

Differentiating a line with respect to the free correlation function removes the line, leaving in a symmetrized way the spatial indices of the free correlation function on the vertices to which the line was connected.

The effect of this derivative is illustrated by studying the diagrammatic effect of the operator

$$\hat{L} = \int_{12} G_{12} \frac{\delta}{\delta G_{12}} \, . \tag{13.31}$$

Applying $\hat{L}$ to a connected vacuum diagram in $W^{(p)}$, the functional derivative $\delta/\delta G_{12}$ removes successively each of its $2p$ lines. Subsequently, the removed lines are again reinserted, so that the connected vacuum diagrams $W^{(p)}$ are eigenfunctions of $\hat{L}$, whose eigenvalues $2p$ count the lines of the diagrams:

$$\hat{L}\, W^{(p)} = 2p\, W^{(p)} . \tag{13.32}$$

As an example, take the explicit first-order expression for the vacuum diagrams, i.e.

$$W^{(1)} = 3 \int_{1234} V_{1234}\, G_{12} G_{34} , \tag{13.33}$$

and apply the basic rule (13.28), leading to the desired eigenvalue 2.

13.3 Perturbation Theory

For the calculation of the vacuum energy $W[0]$ we use functional derivatives with respect to the inverse propagator G^{-1} in the energy functional (13.1) rather than with respect to the current j. This allows us to substitute the previous expression (10.49) for the partition function by

$$Z = \exp\left\{ -\frac{g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right\} e^{W^{(0)}} , \tag{13.34}$$

where the zeroth order of the negative free energy has the diagrammatic representation

$$W^{(0)} = -\frac{1}{2} \operatorname{Tr} \ln G^{-1} \equiv \frac{1}{2} \bigcirc . \tag{13.35}$$

Expanding again the exponential in a power series, we obtain

$$\begin{aligned} Z \;=\; & \left\{ 1 + \frac{-g}{6} \int_{1234} V_{1234} \frac{\delta^2}{\delta G_{12}^{-1} \delta G_{34}^{-1}} \right. & (13.36) \\ & \left. + \frac{1}{2} \left(\frac{-g}{6} \right)^2 \int_{12345678} V_{1234} V_{5678} \frac{\delta^4}{\delta G_{12}^{-1} \delta G_{34}^{-1} \delta G_{56}^{-1} \delta G_{78}^{-1}} + \dots \right\} e^{W^{(0)}} . \end{aligned}$$

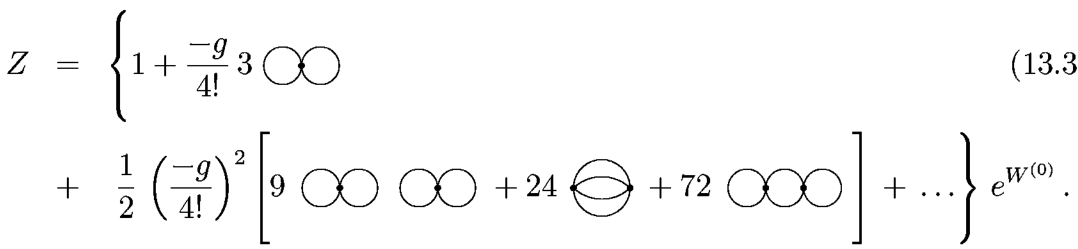
Thus we need only half as many functional derivatives as in the expansion derived with the help of the currents j. Taking into account (13.10), (13.11), and (10.20), we obtain

$$\frac{\delta W^{(0)}}{\delta G_{12}^{-1}} = -\frac{1}{2} G_{12} , \qquad \frac{\delta^2 W^{(0)}}{\delta G_{12}^{-1} \delta G_{34}^{-1}} = \frac{1}{4} \left\{ G_{13} G_{24} + G_{14} G_{23} \right\} , \tag{13.37}$$

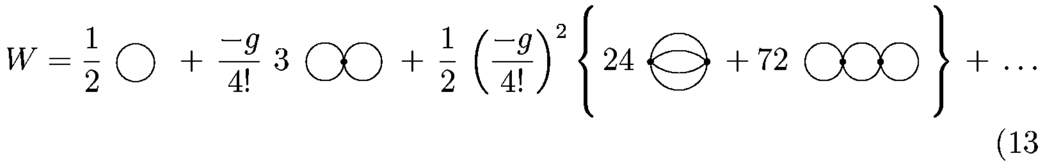
such that the partition function Z becomes

$$\begin{aligned} Z \;=\; & \left\{ 1 + \frac{-g}{4!} 3 \int_{1234} V_{1234}\, G_{12} G_{34} + \frac{1}{2} \left(\frac{-g}{4!} \right)^2 \int_{12345678} V_{1234} V_{5678} \right. & (13.38) \\ & \times \left. \Big[9\, G_{12} G_{34} G_{56} G_{78} + 24\, G_{15} G_{26} G_{37} G_{48} + 72\, G_{12} G_{35} G_{46} G_{78} \Big] + \dots \right\} e^{W^{(0)}} . \end{aligned}$$

This has the diagrammatic representation


(13.39)

All diagrams in this expansion follow directly by successively cutting lines of the basic one-loop vacuum diagram (13.35) according to (13.36). By going to the logarithm of the partition function Z, we find a diagrammatic expansion for the negative free energy W


(13.40)

which turns out to contain precisely all connected diagrams in (13.39) with the same multiplicities. In the next section we show that this diagrammatic expansion for the negative free energy can be derived more efficiently by solving a differential equation.

13.4 Functional Differential Equation for $W = \ln Z$

Regarding the partition function Z as a functional of the inverse propagator G^{-1}, we derive a functional differential equation for Z. We start with the trivial identity

$$\int \mathcal{D}\phi \frac{\delta}{\delta \phi_1} \left\{ \phi_2 \, e^{-E[\phi]} \right\} = 0 \, , \tag{13.41}$$

which follows via functional integration by parts from the vanishing of the exponential at infinite fields. Taking into account the explicit form of the energy functional (13.1), we perform the functional derivative with respect to the field and obtain

$$\int \mathcal{D}\phi \left\{ \delta_{12} - \int_3 G^{-1}_{13} \phi_2 \phi_3 - \frac{g}{6} \int_{345} V_{1345} \, \phi_2 \phi_3 \phi_4 \phi_5 \right\} e^{-E[\phi]} = 0 \, . \tag{13.42}$$

Applying the substitution rule (13.13), this equation can be expressed in terms of the partition function (13.4) and its derivatives with respect to the inverse propagator G^{-1}:

$$\delta_{12} \, Z + 2 \int_3 G^{-1}_{13} \frac{\delta Z}{\delta G^{-1}_{23}} = \frac{2}{3} g \int_{345} V_{1345} \frac{\delta^2 Z}{\delta G^{-1}_{23} \delta G^{-1}_{45}} \, . \tag{13.43}$$

Note that this linear functional differential equation for the partition function Z is, indeed, solved by (13.34) due to the commutation relation

$$\exp\left\{-\frac{g}{6}\int_{1234} V_{1234}\,\frac{\delta^2}{\delta G_{12}^{-1}\delta G_{34}^{-1}}\right\} G_{56}^{-1} - G_{56}^{-1}\exp\left\{-\frac{g}{6}\int_{1234} V_{1234}\,\frac{\delta^2}{\delta G_{12}^{-1}\delta G_{34}^{-1}}\right\}$$
$$= -\frac{g}{3}\int_{78} V_{5678}\,\frac{\delta}{\delta G_{78}^{-1}}\,\exp\left\{-\frac{g}{6}\int_{1234} V_{1234}\,\frac{\delta^2}{\delta G_{12}^{-1}\delta G_{34}^{-1}}\right\} \tag{13.44}$$

which follows from the canonical one

$$\frac{\delta}{\delta G_{12}^{-1}}\,G_{34}^{-1} - G_{34}^{-1}\,\frac{\delta}{\delta G_{12}^{-1}} = \frac{1}{2}\,\{\delta_{13}\delta_{24} + \delta_{14}\delta_{23}\}\,. \tag{13.45}$$

Going over from Z to $W = \ln Z$, the linear functional differential equation (13.43) turns into a nonlinear one:

$$\delta_{12} + 2\int_3 G_{13}^{-1}\,\frac{\delta W}{\delta G_{23}^{-1}} = \frac{2}{3}\,g\int_{345} V_{1345}\left\{\frac{\delta^2 W}{\delta G_{23}^{-1}\delta G_{45}^{-1}} + \frac{\delta W}{\delta G_{23}^{-1}}\,\frac{\delta W}{\delta G_{45}^{-1}}\right\}. \tag{13.46}$$

If the coupling constant g vanishes, this is immediately solved by (13.35). For a nonvanishing coupling constant g, the right-hand side in (13.46) produces corrections to (13.35) which we shall denote with $W^{(\mathrm{int})}$. Thus the negative free energy W decomposes according to

$$W = W^{(0)} + W^{(\mathrm{int})}\,. \tag{13.47}$$

Inserting this into (13.46) and taking into account (13.37), we obtain the following functional differential equation for the interaction negative free energy $W^{(\mathrm{int})}$:

$$\begin{aligned}\int_{12} G_{12}^{-1}\,\frac{\delta W^{(\mathrm{int})}}{\delta G_{12}^{-1}} &= \frac{g}{4}\int_{1234} V_{1234}\,G_{12}G_{34} - \frac{g}{3}\int_{1234} V_{1234}\,G_{12}\,\frac{\delta W^{(\mathrm{int})}}{\delta G_{34}^{-1}}\\ &+ \frac{g}{3}\int_{1234} V_{1234}\left\{\frac{\delta^2 W^{(\mathrm{int})}}{\delta G_{12}^{-1}\delta G_{34}^{-1}} + \frac{\delta W^{(\mathrm{int})}}{\delta G_{12}^{-1}}\,\frac{\delta W^{(\mathrm{int})}}{\delta G_{34}^{-1}}\right\}.\end{aligned} \tag{13.48}$$

With the help of the functional chain rule, the first and second derivatives with respect to the inverse propagator G^{-1} are rewritten as

$$\frac{\delta}{\delta G_{12}^{-1}} = -\int_{34} G_{13}G_{24}\frac{\delta}{\delta G_{34}} \tag{13.49}$$

and

$$\begin{aligned}\frac{\delta^2}{\delta G_{12}^{-1}\delta G_{34}^{-1}} &= \int_{5678} G_{15}G_{26}G_{37}G_{48}\frac{\delta^2}{\delta G_{56}\delta G_{78}} \qquad (13.50)\\ &+ \frac{1}{2}\int_{56}\{G_{13}G_{25}G_{46} + G_{14}G_{25}G_{36} + G_{23}G_{15}G_{46} + G_{24}G_{15}G_{36}\}\,\frac{\delta}{\delta G_{56}}\,,\end{aligned}$$

respectively, so that the functional differential equation (13.48) for $W^{(\mathrm{int})}$ takes the form[5]

$$\int_{12} G_{12}\frac{\delta W^{(\mathrm{int})}}{\delta G_{12}} = -\frac{g}{4}\int_{1234} V_{1234}\,G_{12}G_{34} - g\int_{123456} V_{1234}\,G_{12}G_{35}G_{46}\frac{\delta W^{(\mathrm{int})}}{\delta G_{56}} \qquad (13.51)$$
$$-\frac{g}{3}\int_{12345678} V_{1234}\,G_{15}G_{26}G_{37}G_{48}\left\{\frac{\delta^2 W^{(\mathrm{int})}}{\delta G_{56}\delta G_{78}} + \frac{\delta W^{(\mathrm{int})}}{\delta G_{56}}\frac{\delta W^{(\mathrm{int})}}{\delta G_{78}}\right\}.$$

13.5 Recursion Relation and Graphical Solution

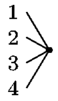
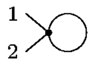
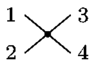
We now convert the functional differential equation (13.51) into a recursion relation by expanding $W^{(\mathrm{int})}$ into a power series in G:

$$W^{(\mathrm{int})} = \sum_{p=1}^{\infty}\frac{1}{p!}\left(\frac{-g}{4!}\right)^p W^{(p)}. \qquad (13.52)$$

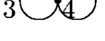
Using the property (13.32) that the coefficient $W^{(p)}$ satisfies the eigenvalue problem of the line numbering operator (13.31), we obtain the recursion relation

$$W^{(\mathrm{p}+1)} = 12\int_{123456} V_{1234}\,G_{12}G_{35}G_{46}\frac{\delta W^{(\mathrm{p})}}{\delta G_{56}} + 4\int_{12345678} V_{1234}\,G_{15}G_{26}G_{37}G_{48}\frac{\delta^2 W^{(\mathrm{p})}}{\delta G_{56}\delta G_{78}}$$
$$+\,4\sum_{q=1}^{p-1}\binom{p}{q}\int_{12345678} V_{1234}\,G_{15}G_{26}G_{37}G_{48}\frac{\delta W^{(\mathrm{p-q})}}{\delta G_{56}}\frac{\delta W^{(\mathrm{q})}}{\delta G_{78}}, \qquad (13.53)$$

and the initial condition (13.33). With the help of the graphical rules of Subsection 13.2, the recursion relation (13.53) can be written diagrammatically as follows

$$W^{(p+1)} = 4\,\frac{\delta^2 W^{(p)}}{\delta 1\text{—}2\;\delta 3\text{—}4}$$

$$+\;12\,\frac{\delta W^{(p)}}{\delta 1\text{—}2}$$

$$+\;4\sum_{q=1}^{p-1}\binom{p}{q}\frac{\delta W^{(p-q)}}{\delta 1\text{—}2}$$

$$\frac{\delta W^{(q)}}{\delta 3\text{—}4},\quad p\geq 1. \qquad (13.54)$$

This is iterated starting from

$$W^{(1)} = 3$$

$$. \qquad (13.55)$$

The right-hand side of (13.54) contains three different graphical operations. The first two are linear and involve one or two line amputations of the previous perturbative order. The third operation is nonlinear and mixes two different one-line amputations of lower orders.

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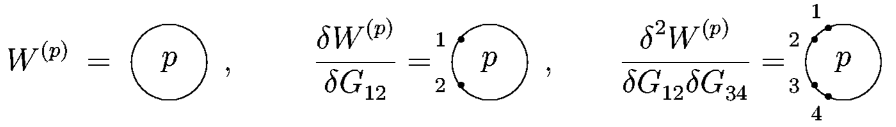
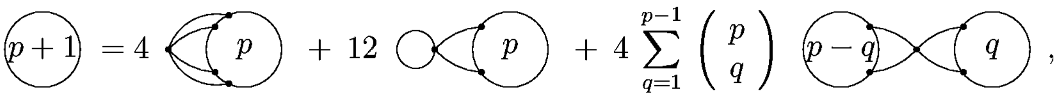
[5] Compare Eq. (51) in the second of the papers quoted in Footnote 1.

An alternative way of formulating the above recursion relation may be based on the graphical rules

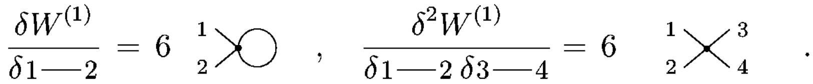

$W^{(p)} =$
p
,
$\frac{\delta W^{(p)}}{\delta G_{12}} =$
1
2
p
,
$\frac{\delta^2 W^{(p)}}{\delta G_{12}\delta G_{34}} =$
1
2
3
4
p
.

(13.56)

With these, the recursion relation (13.54) reads

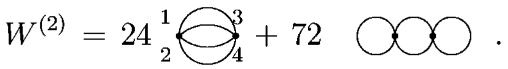

$p+1$
$= 4$
p
$+ 12$
p
$+ 4\sum_{q=1}^{p-1}\binom{p}{q}$
$p-q$
q
,

To demonstrate the working of (13.54), we calculate the connected vacuum diagrams up to five loops. Applying the linear operations to (13.53), we obtain immediately


$\frac{\delta W^{(1)}}{\delta 1\text{—}2} = 6$
1
2
,
$\frac{\delta^2 W^{(1)}}{\delta 1\text{—}2\,\delta 3\text{—}4} = 6$
1
3
2
4
.

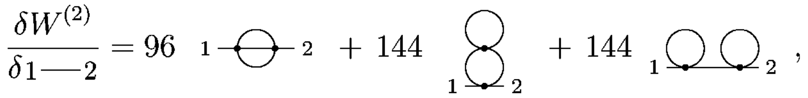
(13.58)

Inserted into (13.54), these lead to the three-loop vacuum diagrams


$W^{(2)} = 24$
1
3
2
4
$+ 72$
.

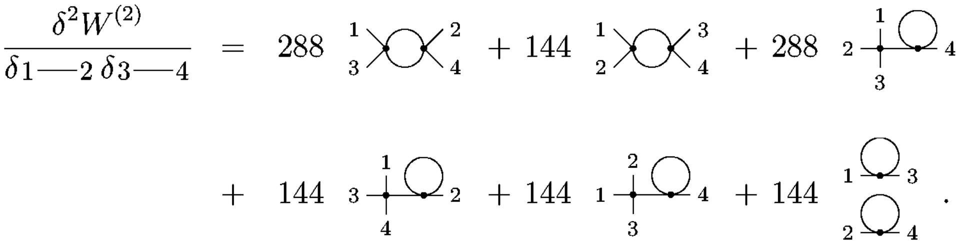
(13.59)

Proceeding to the next order, we have to perform one- and two-line amputations on the vacuum graphs in (13.59), leading to


$\frac{\delta W^{(2)}}{\delta 1\text{—}2} = 96$
1
2
$+ 144$
1
2
$+ 144$
1
2
,

(13.60)

and subsequently to


$\frac{\delta^2 W^{(2)}}{\delta 1\text{—}2\,\delta 3\text{—}4}$
$=$
288
1
2
3
4
$+ 144$
1
3
2
4
$+ 288$
1
2
4
3
$+$
144
1
3
2
4
$+ 144$
2
1
4
3
$+ 144$
1
3
2
4

. (13.61)

Inserting (13.60) and (13.61) into (13.54) and taking into account (13.58), we find the connected vacuum diagrams of order $p = 3$ with their multiplicities as shown in Table 13.1. We observe that the nonlinear operation in (13.54) does not lead to topologically new diagrams. It only corrects the multiplicities of the diagrams generated from the first two operations. This is true also in higher orders. The connected vacuum diagrams of the subsequent order $p = 4$ and their multiplicities are listed in Table 13.1.

As a cross-check we can also determine the total multiplicities $M^{(p)}$ of all connected vacuum diagrams contributing to $W^{(p)}$. To this end we recall that each of the $M^{(p)}$ diagrams in $W^{(p)}$ consists of $2p$ lines. The amputation of one or two lines therefore leads to $2pM^{(p)}$ and $2p(2p-1)M^{(p)}$ diagrams with $2p-1$ and $2p-2$ lines, respectively. Considering only the total multiplicities, the graphical recursion relations (13.54) reduce to the form derived before:[6]

$$M^{(p+1)} = 16p(p+1)M^{(p)} + 16\sum_{q=1}^{p-1} \frac{p!}{(p-q-1)!(q-1)!} M^{(q)} M^{(p-q)}\,; \qquad p \geq 1 \quad (13.62)$$

These are solved starting with the initial value

$$M^{(1)} = 3\,, \tag{13.63}$$

leading to the total multiplicities

$$M^{(2)} = 96\,, \quad M^{(3)} = 9504\,, \quad M^{(4)} = 1880064\,, \tag{13.64}$$

which agree with the results listed in Table 13.1. In addition we note that the next orders would contain

$$M^{(5)} = 616108032\,, \; M^{(6)} = 301093355520\,, \; M^{(7)} = 205062331760640 \tag{13.65}$$

connected vacuum diagrams.

13.6 Scalar $\phi^2 A$-Theory

For the sake of generality, let us also study the situation where the quartic interaction of the ϕ^4-theory is generated by a scalar field A from a cubic $\phi^2 A$-interaction. The associated energy functional

$$E[\phi, A] = E^{(0)}[\phi, A] + E^{(\mathrm{int})}[\phi, A] \tag{13.66}$$

decomposes into the free part

$$E^{(0)}[\phi, A] = \frac{1}{2}\int_{12} G_{12}^{-1}\,\phi_1\phi_2 + \frac{1}{2}\int_{12} H_{12}^{-1}\,A_1 A_2 \tag{13.67}$$

---

[6] See the second of the papers quoted in Footnote 1.

and the interaction

$$E^{(\mathrm{int})}[\phi, A] = \frac{\sqrt{g}}{2} \int_{123} V_{123}\, \phi_1 \phi_2 A_3 \,. \tag{13.68}$$

Indeed, as the field A appears only quadratically in (13.66), the functional integral for the partition function

$$Z = \int \mathcal{D}\phi \mathcal{D}A\, e^{-E[\phi,A]} \tag{13.69}$$

can be exactly evaluated with respect to the field A, yielding

$$Z = \int \mathcal{D}\, e^{-E^{(\mathrm{eff})}[\phi]} \tag{13.70}$$

with the effective energy functional

$$E^{(\mathrm{eff})}[\phi] = -\frac{1}{2} \mathrm{Tr} \ln H^{-1} + \frac{1}{2} \int_{12} G^{-1}_{12}\, \phi_1 \phi_2 - \frac{g}{8} \int_{123456} V_{125} V_{346} H_{56}\, \phi_1 \phi_2 \phi_3 \phi_4 \,. \tag{13.71}$$

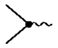
Apart from a trivial shift due to the negative free energy of the field A, the effective energy functional (13.71) coincides with one (13.1) of a ϕ^4-theory with the quartic interaction

$$V_{1234} = -3 \int_{56} V_{125} V_{346} H_{56} \,. \tag{13.72}$$

If we supplement the previous Feynman rules (13.6), (13.8) by the free correlation function of the field A

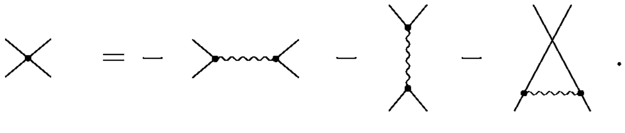
$$1 \sim\!\sim\!\sim 2 \quad \equiv \quad H_{12} \tag{13.73}$$

and the cubic interaction



$$\equiv \quad \int_{123} V_{123} \,, \tag{13.74}$$

the intimate relation (13.72) between the ϕ^4-theory and the $\phi^2 A$- theory can be graphically illustrated by



(13.75)

This corresponds to a photon exchange in the so-called s-, t- and u-channels of Mandelstam's theory of the scattering matrix. Their infinite repetitions yield the relevant forces in the Hartree, Fock and Bogoliubov approximations of many-body physics. In the following we analyze the $\phi^2 A$-theory along similar lines as before the ϕ^4-theory.

13.7 Perturbation Theory

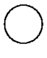
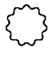
Expanding the exponential in the partition function (13.69) in powers of the coupling constant g, the resulting perturbation series reads

$$Z = \sum_{p=0}^{\infty} \frac{1}{(2p)!} \left(\frac{g}{4}\right)^p \int \mathcal{D}\phi \mathcal{D}A \left(\int_{123456} V_{123} V_{456} \phi_1 \phi_2 \phi_4 \phi_5 A_3 A_6 \right)^p e^{-E^{(0)}[\phi, A]} \,. \qquad (13.76)$$

Substituting the product of two fields ϕ or A by a functional derivative with respect to the inverse propagators G^{-1} or H^{-1}, we conclude from (13.76)

$$Z = \sum_{p=0}^{\infty} \frac{(-2g)^p}{(2p)!} \left(\int_{123456} V_{123} V_{456} \frac{\delta^3}{\delta G_{12}^{-1} \delta G_{45}^{-1} \delta H_{36}^{-1}} \right)^p e^{W^{(0)}} \,, \qquad (13.77)$$

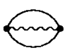
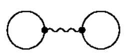
where the zeroth order of the negative free energy reads

$$W^{(0)} = -\frac{1}{2} \mathrm{Tr} \ln G^{-1} - \frac{1}{2} \mathrm{Tr} \ln H^{-1} \equiv \frac{1}{2}$$  $$+ \frac{1}{2}$$  $$. \qquad (13.78)$$

Inserting (13.78) in (13.77), the first-order contribution to the negative free energy yields

$$W^{(1)} = 2 \int_{123456} V_{123} V_{456} \, H_{36} G_{14} G_{25} + \int_{123456} V_{123} V_{456} \, H_{36} G_{12} G_{45} \,, \qquad (13.79)$$

which corresponds to the Feynman diagrams

$$W^{(1)} = 2$$  $$+$$  $$. \qquad (13.80)$$

13.8 Functional Differential Equation for $W = \ln Z$

The derivation of a functional differential equation for the negative free energy W requires the combination of two independent steps. Consider first the identity

$$\int \mathcal{D}\phi \mathcal{D}A \frac{\delta}{\delta \phi_1} \left\{ \phi_2 \, e^{-E[\phi, A]} \right\} = 0 \,, \qquad (13.81)$$

which immediately yields with the energy functional (13.66)

$$\delta_{12} Z + 2 \int_3 G_{13}^{-1} \frac{\delta Z}{\delta G_{23}^{-1}} + 2\sqrt{g} \int_{34} V_{134} \frac{\delta \left\{ \langle A_4 \rangle Z \right\}}{\delta G_{23}^{-1}} = 0 \,, \qquad (13.82)$$

where $\langle A \rangle$ denotes the expectation value of the field A. In order to close the functional differential equation, we consider the second identity

$$\int \mathcal{D}\phi \mathcal{D}A \frac{\delta}{\delta A_1} e^{-E[\phi, A]} = 0 \,, \qquad (13.83)$$

which leads to

$$\langle A_1 \rangle Z = \sqrt{g} \int_{234} V_{234} H_{14} \frac{\delta Z}{\delta G^{-1}_{23}} \,. \tag{13.84}$$

Inserting (13.84) in (13.82), we result in the desired functional differential equation for the negative free energy $W = \ln Z$:

$$\delta_{12} + 2 \int_2 G^{-1}_{13} \frac{\delta W}{\delta G^{-1}_{23}} = -2g \int_{34567} V_{134} V_{567} H_{47} \left\{ \frac{\delta^2 W}{\delta G^{-1}_{23} \delta G^{-1}_{56}} + \frac{\delta W}{\delta G^{-1}_{23}} \frac{\delta W}{\delta G^{-1}_{56}} \right\} . \tag{13.85}$$

A subsequent separation (13.47) of the zeroth order (13.78) leads to a functional differential equation for the interaction part of the free energy $W^{(\mathrm{int})}$:

$$\begin{aligned} \int_{12} G^{-1}_{12} \frac{\delta W^{(\mathrm{int})}}{\delta G^{-1}_{12}} &= -\frac{g}{4} \int_{123456} V_{123} V_{456} H_{36} \left\{ G_{12} G_{45} + 2 G_{14} G_{25} \right\} \\ &\quad + g \int_{123456} V_{123} V_{456} G_{12} H_{36} \frac{\delta W^{(\mathrm{int})}}{\delta G^{-1}_{45}} \\ &\quad - g \int_{123456} V_{123} V_{456} H_{36} \left\{ \frac{\delta^2 W^{(\mathrm{int})}}{\delta G^{-1}_{12} \delta G^{-1}_{45}} + \frac{\delta W^{(\mathrm{int})}}{\delta G^{-1}_{12}} \frac{\delta W^{(\mathrm{int})}}{\delta G^{-1}_{45}} \right\} . \end{aligned} \tag{13.86}$$

Taking into account the functional chain rules (13.49), (13.50), the functional derivatives with respect to G^{-1} in (13.86) can be rewritten in terms of G:

$$\begin{aligned} \int_{12} G_{12} \frac{\delta W^{(\mathrm{int})}}{\delta G_{12}} &= \frac{g}{4} \int_{123456} V_{123} V_{456} H_{36} \left\{ G_{12} G_{45} + 2 G_{14} G_{25} \right\} \\ &\quad + g \int_{123456} V_{123} V_{456} H_{36} \left\{ G_{12} G_{47} G_{58} + 2 G_{14} G_{27} G_{58} \right\} \frac{\delta W^{(\mathrm{int})}}{\delta G_{78}} \\ &\quad + g \int_{1234567891\bar{1}} V_{123} V_{456} H_{36} G_{17} G_{28} G_{39} G_{4\bar{1}} \left\{ \frac{\delta^2 W^{(\mathrm{int})}}{\delta G_{78} \delta G_{9\bar{1}}} + \frac{\delta W^{(\mathrm{int})}}{\delta G_{78}} \frac{\delta W^{(\mathrm{int})}}{\delta G_{9\bar{1}}} \right\} . \end{aligned} \tag{13.87}$$

13.9 Recursion Relation and Graphical Solution

The functional differential equation (13.87) is now solved by the power series

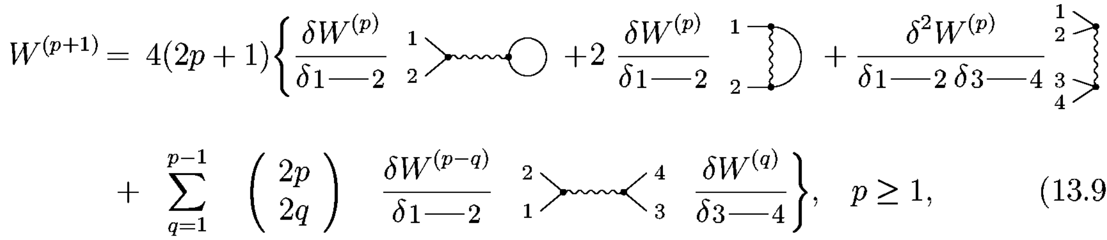
$$W^{(\mathrm{int})} = \sum_{p=1}^{\infty} \frac{1}{(2p)!} \left(\frac{g}{4} \right)^p W^{(p)} \,. \tag{13.88}$$

Using the property (13.32) that the coefficients $W^{(p)}$ satisfy the eigenvalue condition of the operator (13.31), we obtain both the recursion relation

$$W^{(p+1)} = 4(2p+1) \left\{ \int_{12345678} V_{123} V_{456} \, H_{36} \left(G_{12} G_{47} G_{58} + 2 G_{14} G_{27} G_{58} \right) \frac{\delta W^{(p)}}{\delta G_{78}} \right.$$

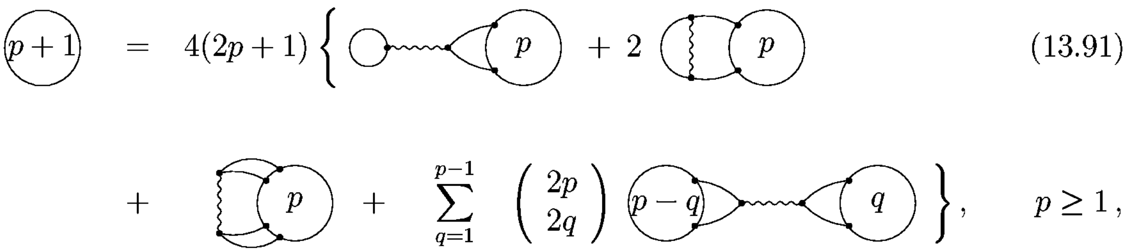
$$+\int_{1234567891\bar{1}} V_{123}V_{456}\,H_{36}G_{17}G_{28}G_{39}G_{4\bar{1}}\left(\frac{\delta^2 W^{(p)}}{\delta G_{78}\delta G_{9\bar{1}}}+\sum_{q=1}^{p-1}\binom{2p}{2q}\frac{\delta W^{(p-q)}}{\delta G_{78}}\,\frac{\delta W^{(q)}}{\delta G_{9\bar{1}}}\right)\Bigg\} \tag{13.89}$$

and the initial value (13.79). Using the Feynman rules (13.6), (13.73) and (13.74), the recursion relation (13.89) reads graphically


$W^{(p+1)} = 4(2p+1)\Big\{\frac{\delta W^{(p)}}{\delta 1\text{---}2}$
1
2
$+2\,\frac{\delta W^{(p)}}{\delta 1\text{---}2}$
1
2
$+\frac{\delta^2 W^{(p)}}{\delta 1\text{---}2\,\delta 3\text{---}4}$
1
2
3
4
$+\sum_{q=1}^{p-1}\binom{2p}{2q}\frac{\delta W^{(p-q)}}{\delta 1\text{---}2}$
2
1
4
3
$\frac{\delta W^{(q)}}{\delta 3\text{---}4}\Big\},\quad p\geq 1,$

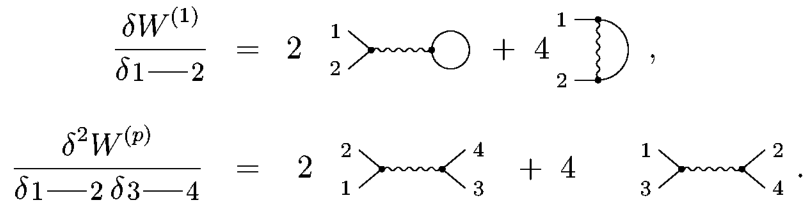
(13.90)

which is iterated starting from (13.80). In analogy to (13.57), this recursion relation can be cast in a closed diagrammatic way by using the alternative graphical rules (13.56):


p + 1
= 4(2p + 1)
p
+ 2
p
+
p
+ $\sum_{q=1}^{p-1}\binom{2p}{2q}$
p − q
q
, p ≥ 1,

(13.91)

We illustrate the procedure of solving the recursion relation (13.90) by construction the three-loop vacuum diagrams. Applying one or two functional derivatives to (13.80), we have


$\frac{\delta W^{(1)}}{\delta 1\text{---}2}$
= 2
1
2
+ 4
1
2
,
$\frac{\delta^2 W^{(p)}}{\delta 1\text{---}2\,\delta 3\text{---}4}$
= 2
2
1
4
3
+ 4
1
3
2
4
.

(13.92)

This is inserted into (13.90) to yield the three-loop diagrams shown in Table 13.4 with their multiplicities. The table also contains the subsequent 4-loop results which we shall not derive here in detail. Observe that the multiplicity of a connected vacuum diagram D in the ϕ^2A-theory is given by a formula similar to (13.9) in the ϕ^4-theory:

$$M^{\rm D}_{\phi^2 A} = \frac{(2p)!4^p}{2!^{S+D}N}\,. \tag{13.93}$$

Here S and D denote the number of self- and double connections, whereas N represents the number of identical vertex permutations.

The connected vacuum diagrams of the ϕ^2A-theory in Table 13.4 can, of course, be converted to corresponding ones of the ϕ^4-theory in Table 13.1, by shrinking wiggly lines to a point and dividing the resulting multiplicity by 3 in accordance with (13.75). This relation between connected vacuum diagrams in ϕ^4- and ϕ^2A-theory is emphasized by the numbering used in Table 13.4. For instance, the shrinking converts the five diagrams #4.1-#4.5 in Table 13.4 to the diagram #4 in Table 13.1. Taking into account the different combinatorial factors in the expansion (13.5) and (13.88) as well as the factor 3 in the shrinkage (13.75), the multiplicity $M_{\phi^4}^{E=0}$ of a ϕ^4-diagram results from the corresponding one $M_{\phi^2A}^{E=0}$ of the ϕ^2A-partner diagrams via the rule

$$M_{\phi^4}^{E=0} = \frac{1}{(2p-1)!!}\, M_{\phi^2A}^{E=0}\,. \tag{13.94}$$

13.10 Computer Generation of Diagrams

Continuing the solution of the graphical recursion relations (13.54) and (13.90) to higher loops becomes an arduous task. We therefore automatize the procedure by computer algebra. Here we restrict ourselves to the ϕ^4-theory because of its relevance for critical phenomena.

13.11 Matrix Representation of Diagrams

To implement the procedure on a computer we must represent Feynman diagrams in the ϕ^4-theory by algebraic symbols. For this we use matrices as defined in the textbook in Footnote 3. Let p be the number of vertices of a given diagram and label them by indices from 1 to p. Set up a matrix $\mathbf{M}$ whose elements M_{ij} $(0 \le i,j \le p)$ specify the number of lines joining the vertices i and j. The diagonal elements M_{ii} $(i > 0)$ count the number of self-connections of the ith vertex. External lines of a diagram are labeled as if they were connected to a single additional dummy vertex with number 0. As matrix element M_{00} is set to zero as a convention. The off-diagonal elements lie in the interval $0 \le M_{ij} \le 4$, while the diagonal elements for $i > 0$ are restricted by $0 \le M_{ii} \le 2$. We observe that the sum of the matrix elements M_{ij} in each row or column equals 4, where the diagonal elements count twice,

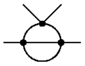
$$\sum_{j=0}^{p} M_{ij} + M_{ii} = \sum_{i=0}^{p} M_{ij} + M_{jj} = 4\,. \tag{13.95}$$

The matrix $\mathbf{M}$ is symmetric and is thus specified by $(p+1)(p+2)/2-1$ elements. Each matrix characterizes a unique diagram and determines its multiplicity via formula (13.27). From the matrix $\mathbf{M}$ we read offdirectly the number of self-, double, triple, fourfold connections S, D, T, F and the number of external legs $E = \sum_{i=1}^{p} M_{0i}$. It also permits us to calculate the number N of identical vertex permutations. For this we observe that the matrix $\mathbf{M}$ is not unique, since so far the vertex numbering is arbitrary. In fact, N is the number of permutations of vertices and external lines which leave the matrix $\mathbf{M}$ unchanged [compare to the statement after (13.27)]. If n_M denotes the number of different matrices representing the same diagram, the number N is given by

$$N = \frac{p!}{n_M} \prod_{i=1}^{p} M_{0i}! \,. \tag{13.96}$$

The matrix elements M_{0i} count the number of external legs connected to the ith vertex. Inserting Eq. (13.96) into the formula (13.27) for $E = 0$, we obtain the multiplicity of the diagram represented by $\mathbf{M}$. This may be used to cross-check the multiplicities obtained before when solving the recursion relation (13.54).

As an example, consider the following diagram of the four-point function with $p = 3$ vertices:

 . (13.97)

This diagram can be represented by altogether $n_M = 3$ different matrices, depending on the labeling of the top vertex with two external legs by 1, 2, or 3:

$$\begin{array}{c|cccc} & 0 & 1 & 2 & 3 \\ \hline 0 & 0 & 2 & 1 & 1 \\ 1 & 2 & 0 & 1 & 1 \\ 2 & 1 & 1 & 0 & 2 \\ 3 & 1 & 1 & 2 & 0 \end{array} \qquad \begin{array}{c|cccc} & 0 & 1 & 2 & 3 \\ \hline 0 & 0 & 1 & 2 & 1 \\ 1 & 1 & 0 & 1 & 2 \\ 2 & 2 & 1 & 0 & 1 \\ 3 & 1 & 2 & 1 & 0 \end{array} \qquad \begin{array}{c|cccc} & 0 & 1 & 2 & 3 \\ \hline 0 & 0 & 1 & 1 & 2 \\ 1 & 1 & 0 & 2 & 1 \\ 2 & 1 & 2 & 0 & 1 \\ 3 & 2 & 1 & 1 & 0 \end{array} \,. \tag{13.98}$$

¿From the zeroth row or column of these matrices or by inspecting the diagram (13.97), we read off that there exist two one-connections and one two-connection between external legs and vertices. Thus Eq. (13.96) states that the number of identical vertex permutations of the diagram (13.97) is 4 (compare the corresponding entry in Table 13.3).

The matrix $\mathbf{M}$ contains of course all information on the topological properties of a diagram. For this we define the submatrix $\tilde{\mathbf{M}}$ by removing the zeroth row and column from $\mathbf{M}$. This allows us to recognize the connectedness of a diagram: A diagram is disconnected if there is a vertex numbering for which $\tilde{\mathbf{M}}$ is a block matrix. Furthermore a vertex is a cutvertex, e.g. a vertex which links two otherwise disconnected parts of a diagram, if the matrix $\tilde{\mathbf{M}}$ has an almost block-form for an appropriate numbering of vertices in which the blocks overlap only on some diagonal element $\tilde{M}_{ii}$, i.e. the matrix $\tilde{\mathbf{M}}$ takes block form if the ith row and column are removed. Similarly, the matrix $\tilde{\mathbf{M}}$ allows us to recognize a one-particle-reducible diagram, which falls into two pieces by cutting a certain line. Removing a line amounts to reducing the associated matrix elements in the submatrix $\tilde{\mathbf{M}}$ by one unit. If the resulting matrix $\tilde{\mathbf{M}}$ has block form, the diagram is one-particle-reducible.

So far, the vertex numbering has been arbitrary, making the matrix representation of a diagram non-unique. To achieve uniqueness, we proceed as follows. We associate with each matrix a number whose digits are composed of the matrix elements M_{ij} $(0 \leq j \leq i \leq p)$, i.e. we form the number with the $(p+1)(p+2)/2-1$ elements

$$M_{10}M_{11}M_{20}M_{21}M_{22}M_{30}M_{31}M_{32}M_{33}\dots M_{pp}\,. \tag{13.99}$$

The smallest of these numbers is chosen to represent the diagram unique. For instance, the three matrices (13.98) carry the numbers

$$201101120\,, \qquad 102101210\,, \qquad 101202110\,, \tag{13.100}$$

the smallest one being the last. Thus we uniquely represent the diagram (13.97) by this number.

13.12 Practical Generation

We are now prepared for the computer generation of Feynman diagrams. First the vacuum diagrams are generated from the recursion relation (13.54). From these the diagrams of the connected two- and four-point functions are obtained by cutting or removing lines. A MATHEMATICA program performs this task. The resulting unique matrix representations of the diagrams up to the order $p=4$ are listed in Table 13.5–13.7. They are the same as those derived before by hand in Table 13.1–13.3. Higher-order results up to $p=6$, containing all diagrams which are relevant for the five loop renormalization of the ϕ^4-theory in $d=4-\epsilon$ dimensions[7] are made available on internet[8], where also the program can be found.

13.12.1 Connected Vacuum Diagrams

The computer solution of the recursion relation (13.54) necessitates to keep an exact record of the labeling of external legs of intermediate diagrams which arise from differentiating a vacuum diagram with respect to a line once or twice. To this end we have to extend our previous matrix representation of diagrams where the external legs are labeled as if they were connected to a simple additional vertex with number 0. For each matrix representing a diagram we define an associated vector which contains the labels of the external legs connected to each vertex. This vector has the length of the dimension of the matrix and will be prepended to the matrix.

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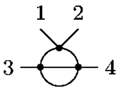
[7] See the textbook in Footnote 3.

[8] http://www.physik.fu-berlin.de/~kleinert/294/programs.

By doing so, it is understood that the rows and columns of the matrix are labeled from 0 to the number of vertices as explained in Subsection IV.A, so that we may omit these labels from now on. Consider, as an example, the diagram (13.97) of the four-point function with $p = 3$ vertices, where the spatial indices $1, 2, 3, 4$ are assigned in a particular order:



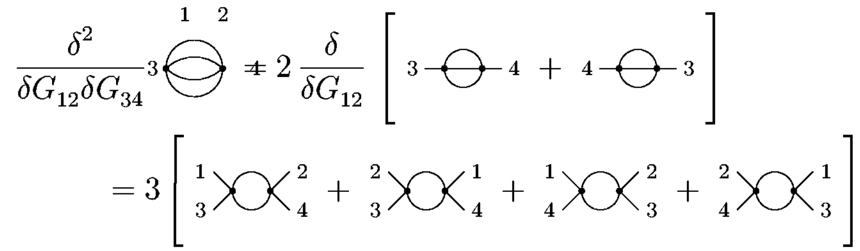
. (13.101)

In our extended matrix notation, such a diagram can be represented in total by six matrices:

$$\left(\begin{array}{c|cccc} \{\} & 0 & 2 & 1 & 1 \\ \{1,2\} & 2 & 0 & 1 & 1 \\ \{3\} & 1 & 1 & 0 & 2 \\ \{4\} & 1 & 1 & 2 & 0 \end{array}\right), \quad \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 2 & 1 \\ \{3\} & 1 & 0 & 1 & 2 \\ \{1,2\} & 2 & 1 & 0 & 1 \\ \{4\} & 1 & 2 & 1 & 0 \end{array}\right), \quad \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 1 & 2 \\ \{3\} & 1 & 0 & 2 & 1 \\ \{4\} & 1 & 2 & 0 & 1 \\ \{1,2\} & 2 & 1 & 1 & 0 \end{array}\right),$$
$$\left(\begin{array}{c|cccc} \{\} & 0 & 2 & 1 & 1 \\ \{1,2\} & 2 & 0 & 1 & 1 \\ \{4\} & 1 & 1 & 0 & 2 \\ \{3\} & 1 & 1 & 2 & 0 \end{array}\right), \quad \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 2 & 1 \\ \{4\} & 1 & 0 & 1 & 2 \\ \{1,2\} & 2 & 1 & 0 & 1 \\ \{3\} & 1 & 2 & 1 & 0 \end{array}\right), \quad \left(\begin{array}{c|cccc} \{\} & 0 & 1 & 1 & 2 \\ \{4\} & 1 & 0 & 2 & 1 \\ \{3\} & 1 & 2 & 0 & 1 \\ \{1,2\} & 2 & 1 & 1 & 0 \end{array}\right). \tag{13.102}$$

In the calculation of the vacuum diagrams from the recursion relation (13.54), starting from the two-loop diagram (13.55), we have to represent three different elementary operations in our extended matrix notation:

1. Taking one or two derivatives of a vacuum diagram with respect to a line. For example, we apply this operation to the vacuum diagram #2 in Table 13.1


$\frac{\delta^2}{\delta G_{12}\delta G_{34}}$
1
2
3
4
= 2 $\frac{\delta}{\delta G_{12}}$
3
4
+
4
3
= 3
1
2
3
4
+
2
1
3
4
+
1
2
4
3
+
2
1
4
3

.(13.103)

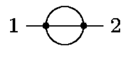
This has the matrix representation

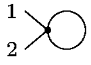
$$\frac{\delta^2}{\delta G_{12}\delta G_{34}} \left(\begin{array}{c|ccc} \{\} & 0 & 0 & 0 \\ \{\} & 0 & 0 & 4 \\ \{\} & 0 & 4 & 0 \end{array}\right) = 2\frac{\delta}{\delta G_{12}} \left[\left(\begin{array}{c|ccc} \{\} & 0 & 1 & 1 \\ \{3\} & 1 & 0 & 3 \\ \{4\} & 1 & 3 & 0 \end{array}\right) + \left(\begin{array}{c|ccc} \{\} & 0 & 1 & 1 \\ \{4\} & 1 & 0 & 3 \\ \{3\} & 1 & 3 & 0 \end{array}\right) \right]$$
$$= 3 \left[\left(\begin{array}{c|ccc} \{\} & 0 & 2 & 2 \\ \{1,3\} & 2 & 0 & 2 \\ \{2,4\} & 2 & 2 & 0 \end{array}\right) + \left(\begin{array}{c|ccc} \{\} & 0 & 2 & 2 \\ \{2,3\} & 2 & 0 & 2 \\ \{1,4\} & 2 & 2 & 0 \end{array}\right) \right]$$

$$+\left(\begin{array}{c|ccc} \{\} & 0 & 2 & 2 \\ \{1,4\} & 2 & 0 & 2 \\ \{2,3\} & 2 & 2 & 0 \end{array}\right) + \left(\begin{array}{c|ccc} \{\} & 0 & 2 & 2 \\ \{2,4\} & 2 & 0 & 2 \\ \{1,3\} & 2 & 2 & 0 \end{array}\right)\Bigg] . \qquad (13.104)$$

The first and fourth matrix as well as the second and third matrix represent the same diagram in (13.103), as can be seen bu permutating rows and columns of either matrix.

2. Combining two or three diagrams to one. We perform this operation by creating a block matrix of internal lines from the submatrices representing the internal lines of the original diagrams. Then the zeroth row or column is added to represent the respective original external spatial arguments. Let us illustrate the combination of two diagrams by the example

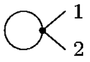


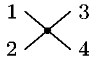


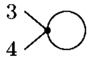
$$\equiv \left(\begin{array}{c|ccc} \{\} & 0 & 1 & 1 \\ \{1\} & 1 & 0 & 3 \\ \{2\} & 1 & 3 & 0 \end{array}\right) , \quad \left(\begin{array}{c|cc} \{\} & 0 & 2 \\ \{1,2\} & 2 & 1 \end{array}\right)$$

$$\to \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 1 & 1 \\ \{1,2\} & 2 & 1 & 0 & 0 \\ \{1\} & 1 & 0 & 0 & 3 \\ \{2\} & 1 & 0 & 3 & 0 \end{array}\right) , \qquad (13.105)$$

and the combination of three diagrams by



,


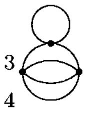
,


$$\equiv \left(\begin{array}{c|cc} \{\} & 0 & 2 \\ \{1,2\} & 2 & 1 \end{array}\right) , \left(\begin{array}{c|cc} \{\} & 0 & 4 \\ \{1,2,3,4\} & 4 & 0 \end{array}\right) , \left(\begin{array}{c|cc} \{\} & 0 & 2 \\ \{3,4\} & 2 & 1 \end{array}\right)$$

$$\to \left(\begin{array}{c|cccc} \{\} & 0 & 2 & 4 & 2 \\ \{1,2\} & 2 & 1 & 0 & 0 \\ \{1,2,3,4\} & 4 & 0 & 0 & 0 \\ \{3,4\} & 2 & 0 & 0 & 1 \end{array}\right) . \qquad (13.106)$$

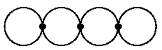
We observe that the ordering of the submatrices in the block matrix is arbitrary at this point, we just have to make sure to distribute the spatial labels of the external legs correctly.

3. Connecting external legs with the same label and creating an internal line. This is achieved in our extended matrix notation by eliminating the spatial labels of external legs which appear twice, and by performing an appropriate entry in the matrix for the additional line. Thus we obtain, for instance, from (13.105)



$$\equiv \left(\begin{array}{c|cccc} \{\} & 0 & 0 & 0 & 0 \\ \{\} & 0 & 1 & 1 & 1 \\ \{\} & 0 & 1 & 0 & 3 \\ \{\} & 0 & 1 & 3 & 0 \end{array}\right) \qquad (13.107)$$

and similarily from (13.106)



$$\equiv \left(\begin{array}{c|cccc} \{\} & 0 & 0 & 0 & 0 \\ \{\} & 0 & 1 & 2 & 0 \\ \{\} & 0 & 2 & 0 & 2 \\ \{\} & 0 & 0 & 2 & 1 \end{array}\right). \tag{13.108}$$

As we reobtain at this stage connected vacuum diagrams where there are no more external legs to be labeled, we may omit the prepended vector.

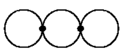
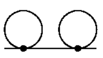
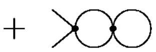
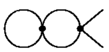
The selection of a unique matrix representation for the resulting vacuum diagrams obtained at each stage of the recursion relation proceeds as explained in detail in Subsection IV.A. By comparing we find out which of the vacuum diagrams are topologically identical and sum up their individual multiplicities. Along these lines, the recursion relation (13.54) is solved by a MATHEMATICA program up to the order $p = 6$. The results are shown in Table 13.5, available on the internet at the address stated in Footnote 8. To each order p, the numbers $n_p^{(0)}$ of topologically different connected vacuum diagrams are

p	1	2	3	4	5	6
$n_p^{(0)}$	1	2	4	10	28	97

(13.109)

13.12.2 Two- and Four-Point Functions $\mathbf{G}_{12}$ and $\mathbf{G}^c_{1234}$ from Cutting Lines

Having found all connected vacuum diagrams, we derive from these the diagrams of the connected two- and four-point functions by using the relations (13.17) and (13.24). In the matrix representation, cutting a line is essentially identical to removing a line as explained above, except that we now interpret the labels which represent the external spatial labels as sitting on the end of lines. Since we are not going to distinguish between trivially "crossed" graphs which are related by exchanging external labels in our computer implementation, we need no longer carry around external spatial labels. Thus we omit the additional vector prepended to the matrix representing a diagram when generating vacuum diagrams. As an example, consider cutting a line in diagram #3 in Table 13.1

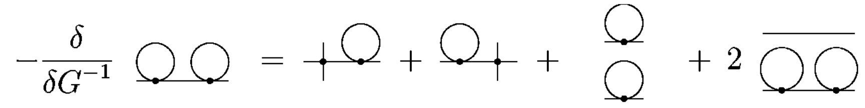
$$-\frac{\delta}{\delta G^{-1}}$$  $$= 2$$  $$+$$  $$+$$  , (13.110)

which has the matrix representation

$$-\frac{\delta}{\delta G^{-1}}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 2 & 1 \end{pmatrix} = 2\begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 2 \\ 0 & 2 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 2 \\ 0 & 1 & 2 \\ 2 & 2 & 0 \end{pmatrix}. \tag{13.111}$$

Here the plus signs and multiplication by 2 have a set-theoretical meaning and are not to be understood as matrix algebra operations. The last two matrices represent, incidentally, the same graph in (13.110) as can be seen by exchanging the last two rows and columns of either matrix.

To create the connected four-point function, we also have to consider second derivatives of vacuum diagrams with respect to G^{-1}. If an external line is cut, an additional external line will be created which is not connected to any vertex. It can be interpreted as a self-connection of the zeroth vertex which collects the external lines. This may be accomodated in the matrix notation by letting the matrix element M_{00} count the number of lines not connected to any vertex. For example, taking the derivative of the first diagram in Eq. (13.110) gives



(13.112)

with the matrix notation

$$-\frac{\delta}{\delta G^{-1}}\begin{pmatrix}0&1&1\\1&1&1\\1&1&1\end{pmatrix}=\begin{pmatrix}0&3&1\\3&0&1\\1&1&1\end{pmatrix}+\begin{pmatrix}0&1&3\\1&1&1\\3&1&0\end{pmatrix}+\begin{pmatrix}0&2&2\\2&1&0\\2&0&1\end{pmatrix}+2\begin{pmatrix}1&1&1\\1&1&1\\1&1&1\end{pmatrix}. \tag{13.113}$$

The first two matrices represent the same diagram as can be seen from Eq. (13.112). The last two matrices in Eq. (13.113) correspond to disconnected diagrams: the first because of the absence of a connection between the two vertices, the second because of the disconnected line represented by the entry $M_{00} = 1$. In the full expression for the two loop contribution $G^{c,(2)}_{1234}$ to the four-point function in Eq. (13.24) all disconnected diagrams arising from cutting a line in $G^{(2)}_{12}$ are canceled by diagrams resulting from the sum. Therefore we may omit the sum, take only the first term and discard all disconnected graphs it creates. This is particularly useful for treating low orders by hand. If we include the sum, we use the prescription of combining diagrams into one as described above in Subsection IV.B.1, except that we now omit the extra vector with the labels of spatial arguments.

13.12.3 Two- and Four-Point Function $\mathbf{G}_{12}$ and $\mathbf{G}^c_{1234}$ from Removing Lines

Instead of cutting lines of connected vacuum graphs once or twice, the perturbative coefficients of $\mathbf{G}_{12}$ and $\mathbf{G}^c_{1234}$ can also be obtained graphically by removing lines. Indeed, from (13.15), (13.37), (13.47) and (13.49) we get for the two-point function

$$\mathbf{G}_{12} = G_{12} + 2\int_{34} G_{13}G_{24}\frac{\delta W^{(\mathrm{int})}}{\delta G_{34}}\,, \tag{13.114}$$

so that we have for $p > 0$

$$\mathbf{G}_{12}^{(p)} = 2 \int_{34} G_{13} G_{24} \frac{\delta W^{(p)}}{\delta G_{34}} \tag{13.115}$$

at our disposal to compute the coefficients $\mathbf{G}_{12}^{(p)}$ from removing one line in the connected vacuum diagrams $W^{(p)}$ in all possible ways. The corresponding matrix operations are identical to the ones for cutting a line so that in this respect there is no difference between both procedures to obtain $\mathbf{G}_{12}$.

Combining (13.114) with (13.11), (13.22) and (13.49), we get for the connected four-point function

$$\begin{aligned}\mathbf{G}_{1234}^{c} &= 4 \int_{5678} G_{15} G_{26} G_{37} G_{48} \frac{\delta^2 W^{(\mathrm{int})}}{\delta G_{56} \delta G_{78}} \\ &- 4 \int_{5678} G_{15} G_{27} (G_{36} G_{48} + G_{46} G_{38}) \frac{\delta W^{(\mathrm{int})}}{\delta G_{56}} \frac{\delta W^{(\mathrm{int})}}{\delta G_{78}},\end{aligned} \tag{13.116}$$

which is equivalent to

$$\begin{aligned}\mathbf{G}_{1234}^{c,(p)} &= 4 \int_{5678} G_{15} G_{26} G_{37} G_{48} \frac{\delta^2 W^{(p)}}{\delta G_{56} \delta G_{78}} \\ &- 4 \sum_{q=1}^{p-1} \binom{p}{q} \int_{5678} G_{15} G_{27} (G_{36} G_{48} + G_{46} G_{38}) \frac{\delta W^{(q)}}{\delta G_{56}} \frac{\delta W^{(p-q)}}{\delta G_{78}}.\end{aligned} \tag{13.117}$$

Again, the sum serves only to subtract disconnected diagrams which are created by the first term, so we may choose to discard both in the first term.

Now the problem of generating diagrams is reduced to the generation of vacuum diagrams and subsequently taking functional derivatives with respect to G_{12}. An advantage of this approach is that external lines do not appear at intermediate steps. So when one uses the cancellation of disconnected terms as a cross check, there are less operations to be performed than with cutting. At the end one just interprets external labels as sitting on external lines. Since all necessary operations on matrices have already been introduced, we omit examples here and just note that we can again omit external labels if we are not distinguishing between trivially "crossed" graphs.

The generation of diagrams of the connected two- and four-point functions has been implemented in both possible ways. Cutting or removing one or two lines in the connected vacuum diagrams up to the order $p = 6$ lead to the following numbers $n_p^{(2)}$ and $n_p^{(2)}$ of topologically different diagrams of $\mathbf{G}_{12}^{(p)}$ and $\mathbf{G}_{1234}^{c,(p)}$:

p	1	2	3	4	5	6
$n_p^{(2)}$	1	3	8	30	118	548
$n_p^{(4)}$	1	2	8	37	181	1010

(13.118)

TABLE 13.1 Connected vacuum diagrams and their multiplicities of the ϕ^4-theory up to five loops. Each diagram is characterized by the vector $(S, D, T, F; N)$ whose components specify the number of self-, double, triple and fourfold connections, and of the identical vertex permutations, respectively.

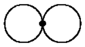
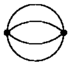
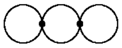
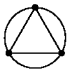
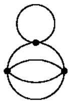
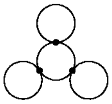
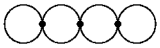
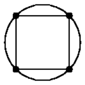
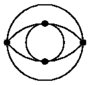
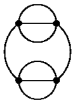
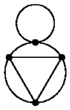
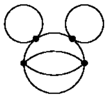
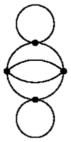
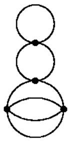
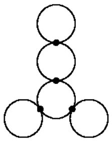
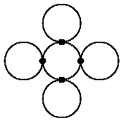
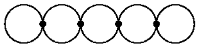
p	$W^{(p)}$
1	#1 3 (2,1,0,0;1) 
2	#2 24 (0,0,0,1;2)  #3 72 (2,1,0,0;2) 
3	#4 1728 (0,3,0,0;6)  #5 3456 (1,0,1,0;2)  #6 1728 (3,0,0,0;6)  #7 2592 (2,2,0,0;2) 
4	#8 62208 (0,4,0,0;8)  #9 248832 (0,2,0,0;8)  #10 55296 (0,0,2,0;4)  #11 497664 (1,2,0,0;2)  #12 165888 (2,0,1,0;2)  #13 248832 (2,1,0,0;4)  #14 165888 (1,1,1,0;2)  #15 248832 (3,1,0,0;2)  #16 62208 (4,0,0,0;8)  #17 124416 (2,3,0,0;2) 

Table 13.2 Connected diagrams of the two-point function and their multiplicities of the ϕ^4-theory up to four loops. Each diagram is characterized by the vector $(S, D, T; N)$ whose components specify the number of self-, double, triple connections, and of the identical vertex permutations, respectively.

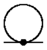
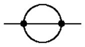
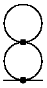
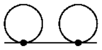
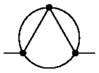
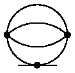
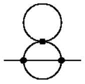
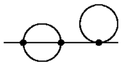
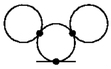
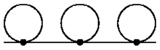
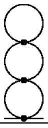
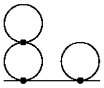
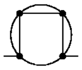
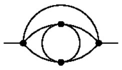
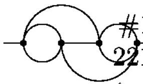
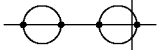
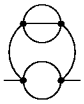
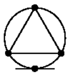
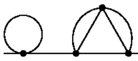
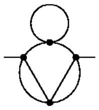
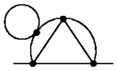
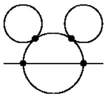
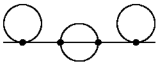
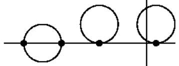
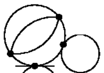
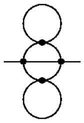
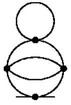
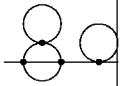
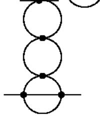
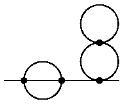
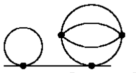
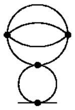
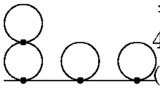
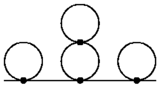
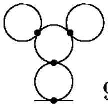
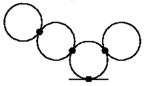
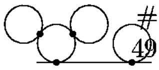
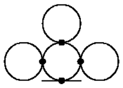
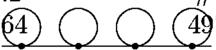
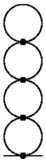
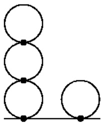
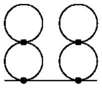
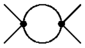
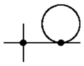
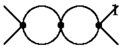
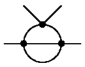
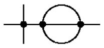
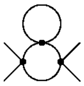
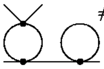
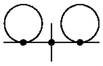
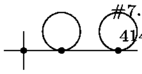
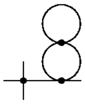
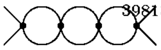
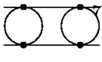
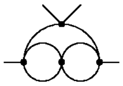
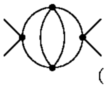
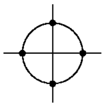
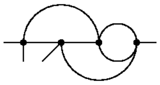
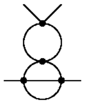
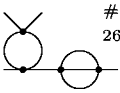
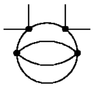
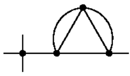
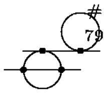
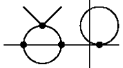
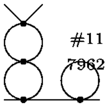
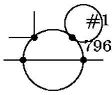
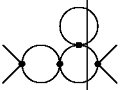
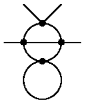
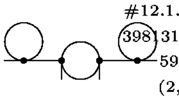
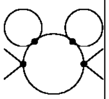
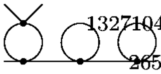
p	$\mathbf{G}_{12}^{(p)}$
1	#1.1 12 (1,0,0;2) 
2	#2.1 192 (0,0,1;2)  #3.1 288 (1,1,0;2)  #3.2 288 (2,0,0;2) 
3	#4.1 20736 (0,2,0;2)  #5.1 6912 (0,0,1;4)  #5.2 20736 (1,1,0;2)  #5.3 13824 (1,0,1;1) 
	#6.1 10368 (2,0,0;4)  #6.2 10368 (3,0,0;2)  #7.1 10368 (1,2,0;2)  #7.2 20736 (2,1,0;1) 
4	#8.1 995328 (0,3,0;2)  #9.1 1990656 (0,1,0;4)  #9.2 1990656 (0,2,0;2)  #10.1 221184 (0,0,2;2)  #10.2 663552 (0,1,1;2)  #11.1 995328 (0,2,0;4)  #11.2 1990656 (1,2,0;1)  #11.3 995328 (1,2,0;2)  #11.4 3981312 (1,1,0;1)  #12.1 995328 (2,1,0;2)  #12.2 331776 (2,0,1;2)  #12.3 663552 (2,0,1;1)  #12.4 663552 (1,0,1;2)  #13.1 995328 (2,0,0;4)  #13.2 995328 (1,1,0;4)  #13.3 1990656 (2,1,0;1)  #14.1 995328 (1,2,0;2)  #14.2 663552 (1,1,1;1)  #14.3 663552 (1,0,1;2)  #14.4 331776 (0,1,1;4)  #15.1 995328 (3,1,0;1)  #15.2 497664 (3,1,0;2)  #15.3 497664 (2,1,0;4)  #15.4 995328 (2,1,0;2)  #15.5 995328 (3,0,0;2)  #16.1 497664 (3,0,0;4)  #16.2 497664 (4,0,0;2)  #17.1 497664 (1,3,0;2)  #17.2 995328 (2,2,0;1)  #17.3 497664 (2,2,0;2) 

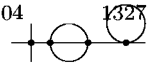
TABLE 13.3 Connected diagrams of the four-point function and their multiplicities of the ϕ^4-theory up to three loops. Each diagram is characterized by the vector $(S, D, T; N)$ whose components specify the number of self-, double, triple connections, and of the identical vertex permutations, respectively.

p	$\mathbf{G}^{c,(p)}_{1234}$
1	#1.1.1 24 (0,0,0;24)
2	#2.1.1,#3.1.1 1152,576 1728 (0,1,0;8) 
	#3.1.2,#3.2.1 1152,1152 2304 (1,0,0;6) 
3	#4.1.1,#7.1.1 41472,20736 62208 (0,2,0;8) 
	#4.1.2,#5.1.1,#5.2.1 165888,41472,41472 248832 (0,1,0;4) 
	#5.1.2,#5.3.2 27648,27648 55296 (0,0,1;6) 
	#5.2.2,#6.1.1 82944,41472 124416 (1,0,0;8) 
	#5.2.3,#5.3.1,#7.1.2,#7.2.1 82944,82944,41472,41472 248832 (1,1,0;2) 
	#6.1.2,#6.2.2,#7.2.2 20736,20736,82944 124416 (2,0,0;4) 
	#6.1.3,#6.2.1 41472,41472 82944 (2,0,0;6) 
	#7.1.3,#7.2.3 41472,41472 82944 (1,1,0;6) 
4	#8.1.1,#17.1.1 1990656,995328 2985984 (0,3,0;8) 
	#8.1.2,#9.2.1,#10.2.1 3981312,3981312,3981312 11943936 (0,2,0;4) 
	#8.1.3,#11.1.2,#11.3.1 7962624,1990656,1990656 11943936 (0,2,0;4) 
	#9.1.1,#13.2.1 3981312,1990656 5971968 (0,1,0;16) 
	#9.1.2 7962624 (0,0,0;24) 
	#9.1.3,#9.2.3,#11.1.1,#11.4.1 15925248,15925248,7962624,7962624 47775744 (0,1,0;2) 
	#9.2.2,#14.1.1,#14.4.3 7962624,1990656,1990656 11943936 (0,2,0;4) 
	#10.1.1,#10.2.3,#14.2.1,#14.4.2 2654208,2654208,1327104,1327104 7962624 (0,1,1;2) 
	#10.2.2,#12.4.1 2654208,1327104 3981312 (0,0,1;8) 
	#11.1.3,#11.2.1 3981312,3981312 7962624 (0,2,0;6) 
	#11.2.2,#11.4.3,#14.1.2,#14.3.3 7962624,7962624,3981312,3981312 23887872 (1,1,0;2) 
	#11.2.3,#11.4.2,#13.2.2,#13.3.1 7962624,7962624,3981312,3981312 23887872 (1,1,0;2) 
	#11.2.4,#11.3.2,#17.1.2,#17.2.1 3981312,3981312,1990656,1990656 11943936 (1,2,0;2) 
	#11.3.3,#11.4.4,#12.1.1,#12.4.5 7962624,7962624,3981312,3981312 23887872 (1,1,0;2) 
	#11.4.5,#15.3.1,#15.4.1 7962624,1990656,1990656 11943936 (1,1,0;4) 
	#11.4.6,#13.1.1,#13.2.3 15925248,3981312,3981312 23887872 (1,0,0;4) 
	#12.1.2,#12.2.2,#13.3.3,#17.2.2 1990656,1990656,3981312,3981312 11943936 (2,1,0;2) 
	#12.1.3,#16.1.2 3981312,1990656 5971968 (2,0,0;8) 

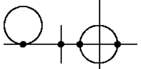
#12.1.4,#12.3.3,#15.1.1,#15.3.2
3981312,3981312,1990656,1990656
11943936
(2,1,0;2)



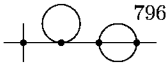
#12.2.1,#12.4.2
1327104,1327104
2654208
(1,0,1;6)



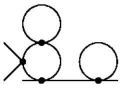
#12.3.2,#12.4.3,#14.2.2,#14.3.2
1327104,1327104,2654208,2654208
7962624
(1,0,1;2)



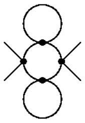
#12.3.1,#12.4.4
1327104,1327104
2654208
(1,0,1;6)



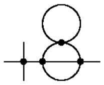
#13.1.2,#13.3.4,#15.4.2,#15.5.1
7962624,7962624,3981312,3981312
23887872
(2,0,0;2)



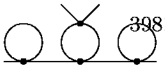
#13.1.3,#16.1.1
1990656,995328
2985984
(2,0,0;16)



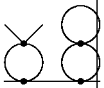
#13.2.4,#13.3.5
3981312,3981312
7962624
(1,1,0;6)



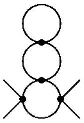
#13.3.2,#15.2.1,#15.3.3
3981312,995328,995328
5971968
(2,1,0;4)



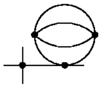
#14.1.3,#14.2.3,#17.1.3,#17.3.1
3981312,3981312,1990656,1990656
11943936
(1,2,0;2)



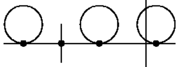
#14.1.4,#15.4.4
3981312,1990656
5971968
(1,1,0;8)



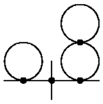
#14.3.1,#14.4.1
1327104,1327104
2654208
(0,0,1;12)



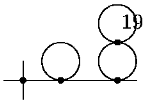
#15.1.2,#15.5.3,#16.1.3,#16.2.2
3981312,3981312,1990656,1990656
11943936
(3,0,0;2)



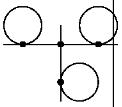
#15.1.3,#15.4.3,#17.2.3,#17.3.2
1990656,1990656,3981312,3981312
11943936
(2,1,0;2)



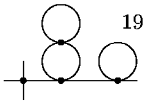
#15.1.4,#15.4.5
1990656,1990656
3981312
(2,1,0;6)



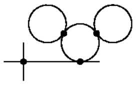
#15.2.2,#15.5.2
1990656,1990656
3981312
(3,0,0;6)



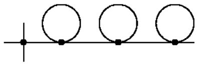
#15.2.3,#15.4.6
1990656,1990656
3981312
(2,1,0;6)



#15.3.4,#15.5.4
1990656,1990656
3981312
(2,0,0;12)



#16.1.4,#16.2.1
1990656,1990656
3981312
(3,0,0;6)



#17.1.4,#17.2.4
1990656,1990656
3981312
(1,2,0;6)

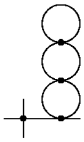


TABLE 13.4 Connected vacuum diagrams and their multiplicities of the $\phi^2 A$-theory up to four loops. Each diagram is characterized by the vector $(S, D; N)$ whose components specify the number of self- and double connections as well as the identical vertex permutations, respectively.

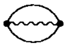
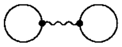
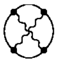
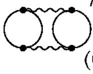
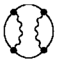
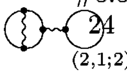
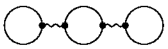
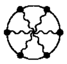
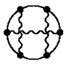
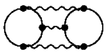
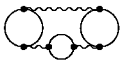
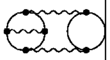
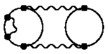
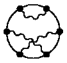
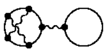
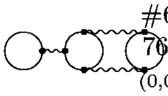
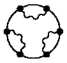
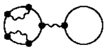
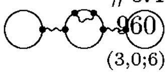
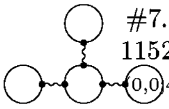
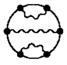
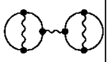
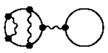
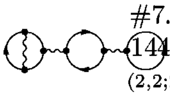
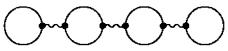
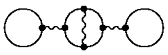
p	$W^{(p)}$
1	#1.1 2 (0,1;2)  #1.2 1 (2,0;2) 
2	#2.1 48 (0,0;8)  #2.2 24 (0,2;4)  #3.1 96 (0,0;4)  #3.2 96 (1,0;2)  #3.3 24 (2,1;2) 
3	#4.1 3840 (0,0;12)  #4.2 11520 (0,0;4)  #4.3 3840 (0,0;12)  #4.4 960 (0,3;6)  #4.5 5760 (0,1;4)  #5.1 11520 (0,1;2)  #5.2 23040 (0,0;2)  #5.3 11520 (1,0;2)  #5.4 5760 (1,1;2)  #6.1 7680 (0,0;6)  #6.2 11520 (1,0;2)  #6.3 5760 (2,0;2)  #6.4 960 (3,0;6)  #7.1 11520 (0,0;4)  #7.2 5760 (0,0;8)  #7.3 11520 (1,0;2)  #7.4 5760 (1,1;2)  #7.5 1440 (2,2;2)  #7.6 2880 (2,0;4) 

TABLE 13.5 Unique matrix representation of all connected vacuum diagrams of ϕ^4-theory up to the order $p = 4$. The number in the first column corresponds to their graphical representation in Table 13.1. The matrix elements M_{ij} represent the numbers of lines connecting two vertices i and j, with omitting $M_{i0} = 0$ for simplicity. The running numbers of the vertices are listed on top of each column in the first two rows. The further columns contain the vector $(S, D, T, F; N)$ characterizing the topology of the diagram, the multiplicity M and the weight $W = M/(4!)^p p!$.

$W^{(1)}$: 1 diagram				
i	1			
j	1			
#	M_{ij}	$(S,D,T,F;N)$	M	W^{-1}
1	2	(2,1,0,0;1)	3	8

$W^{(2)}$: 2 diagrams					
i	1	22			
j	1	12			
#	M_{ij}		$(S,D,T,F;N)$	M	W^{-1}
2	0	40	(0,0,0,1;2)	24	48
3	1	21	(2,1,0,0;2)	72	16

$W^{(3)}$: 4 diagrams						
i	1	22	333			
j	1	12	123			
#	M_{ij}			$(S,D,T,F;N)$	M	W^{-1}
5	0	11	310	(1,0,1,0;2)	3456	24
4	0	20	220	(0,3,0,0;6)	1728	48
7	0	21	201	(2,2,0,0;2)	2592	32
6	1	11	111	(3,0,0,0;6)	1728	48

$W^{(4)}$: 10 diagrams							
i	1	22	333	4444			
j	1	12	123	1234			
#	M_{ij}				$(S,D,T,F;N)$	M	W^{-1}
10	0	00	130	3100	(0,0,2,0;4)	55296	144
8	0	00	220	2200	(0,4,0,0;8)	62208	128
12	0	01	111	3100	(2,0,1,0;2)	165888	48
14	0	01	120	3010	(1,1,1,0;2)	165888	48
17	0	01	201	2200	(2,3,0,0;2)	124416	64
11	0	01	210	2110	(1,2,0,0;2)	497664	16
9	0	10	120	2110	(0,2,0,0;8)	248832	32
13	0	11	101	2110	(2,1,0,0;4)	248832	32
15	0	11	111	2001	(3,1,0,0;2)	248832	32
16	1	01	111	1101	(4,0,0,0;8)	62208	128

TABLE 13.6 Unique matrix representation of all connected two-point function of ϕ^4-theory up to the order $p = 4$. The numbers in the first column correspond to their graphical representation in Table 13.2. The matrix elements M_{ij} represent the numbers of lines connecting two vertices i and j, with omitting $M_{i0} = 0$ for simplicity. The running numbers of the vertices are listed on top of each column in the first two rows. The further columns contain the vector $(S, D, T; N)$ characterizing the topology of the diagram, the multiplicity M and the weight $W = M/(4!)^p p!$.

$\mathbf{G}^{(1)}_{12}$: 1 diagram				
i	11			
j	01			
#	M_{ij}	$(S,D,T;N)$	M	W^{-1}
1.1	21	(1,0,0;2)	12	4

$\mathbf{G}^{(2)}_{12}$: 3 diagrams					
i	11	222			
j	01	012			
#	M_{ij}		$(S,D,T;N)$	M	W^{-1}
3.1	01	220	(1,1,0;2)	288	8
2.1	10	130	(0,0,1;2)	192	12
3.2	11	111	(2,0,0;2)	288	8

$\mathbf{G}^{(3)}_{12}$: 8 diagrams						
i	11	222	3333			
j	01	012	0123			
#	M_{ij}			$(S,D,T;N)$	M	W^{-1}
7.1	00	021	2200	(1,2,0;2)	10368	16
5.1	00	030	2110	(0,0,1;4)	6912	24
5.3	00	111	1300	(1,0,1;1)	13824	12
4.1	00	120	1210	(0,2,0;2)	20736	8
6.1	01	011	2110	(2,0,0;4)	10368	16
7.2	01	101	1210	(2,1,0;1)	20736	8
5.2	01	110	1120	(1,1,0;2)	20736	8
6.2	01	111	1101	(3,0,0;2)	10368	16

$\mathbf{G}^{(4)}_{12}$: 30 diagrams							
i	11	222	3333	44444			
j	01	012	0123	01234			
#	M_{ij}				$(S,D,T;N)$	M	W^{-1}
17.1	00	001	0220	22000	(1,3,0;2)	497664	32
12.4	00	001	0310	21100	(1,0,1;2)	663552	24
14.2	00	001	1120	13000	(1,1,1;1)	663552	24
11.3	00	001	1210	12100	(1,2,0;2)	995328	16
14.4	00	010	0130	22000	(0,1,1;4)	331776	48
11.1	00	010	0220	21100	(0,2,0;4)	995328	16
10.1	00	010	1030	13000	(0,0,2;2)	221184	72
9.2	00	010	1120	12100	(0,2,0;2)	1990656	8
15.3	00	011	0111	22000	(2,1,0;4)	497664	32
15.4	00	011	0201	21100	(2,1,0;2)	995328	16
13.2	00	011	0210	21010	(1,1,0;4)	995328	16
12.3	00	011	1011	13000	(2,0,1;1)	663552	24
13.3	00	011	1101	12100	(2,1,0;1)	1990656	8
11.4	00	011	1110	12010	(1,1,0;1)	3981312	4
11.2	00	020	1011	12100	(1,2,0;1)	1990656	8
8.1	00	020	1020	12010	(0,3,0;2)	995328	16
9.1	00	020	1110	11110	(0,1,0;4)	1990656	8
17.2	00	021	1001	12010	(2,2,0;1)	995328	16
14.1	00	021	1100	11020	(1,2,0;2)	995328	16
15.2	00	021	1101	11001	(3,1,0;2)	497664	32
14.3	00	030	1001	11110	(1,0,1;2)	663552	24
10.2	00	030	1010	11020	(0,1,1;2)	663552	24
12.2	00	030	1011	11001	(2,0,1;2)	331776	48
16.1	01	001	0111	21100	(3,0,0;4)	497664	32
15.1	01	001	1011	12100	(3,1,0;1)	995328	16
17.3	01	001	1020	12010	(2,2,0;2)	497664	32
13.1	01	001	1110	11110	(2,0,0;4)	995328	16
15.5	01	011	1001	11110	(3,0,0;2)	995328	16
12.1	01	011	1010	11020	(2,1,0;2)	995328	16
16.2	01	011	1011	11001	(4,0,0;2)	497664	32

TABLE 13.7 Unique matrix representation of all connected two-point function of ϕ^4-theory up to the order $p = 4$. The numbers in the first column correspond to their graphical representation in Table 13.3. The matrix elements M_{ij} represent the numbers of lines connecting two vertices i and j, with omitting $M_{i0} = 0$ for simplicity. The running numbers of the vertices are listed on top of each column in the first two rows. The further columns contain the vector $(S, D, T; N)$ characterizing the topology of the diagram, the multiplicity M and the weight $W = M/(4!)^p p!$.

$\mathbf{G}^{c,(1)}_{1234}$: 1 diagram				
i	11			
j	01			
#	M_{ij}	$(S,D,T;N)$	M	W^{-1}
1.1.1	40	(0,0,0;24)	24	24

$\mathbf{G}^{c,(2)}_{1234}$: 2 diagrams					
i	11	222			
j	01	012			
#	M_{ij}		$(S,D,T;N)$	M	W^{-1}
3.1.2, 3.2.1	11	310	(1,0,0;6)	2304	12
2.1.1, 3.1.1	20	220	(0,1,0;8)	1728	16

$\mathbf{G}^{c,(3)}_{1234}$: 8 diagrams						
i	11	222	3333			
j	01	012	0123			
#	M_{ij}			$(S,D,T;N)$	M	W^{-1}
5.1.2, 5.3.2	00	130	3100	(0,0,1;6)	55296	36
4.1.1, 7.1.1	00	220	2200	(0,2,0;8)	62208	32
6.1.3, 6.2.1	01	111	3100	(2,0,0;6)	82944	24
7.1.3, 7.2.3	01	120	3010	(1,1,0;6)	82944	24
5.2.2, 6.1.1	01	210	2110	(1,0,0;8)	124416	16
5.2.3, 5.3.1, 7.1.2, 7.2.1	10	111	2200	(1,1,0;2)	248832	8
4.1.2, 5.1.1, 5.2.1	10	120	2110	(0,1,0;4)	248832	8
6.1.2, 6.2.2, 7.2.2	11	101	2110	(2,0,0;4)	124416	16

$\mathbf{G}^{c,(4)}_{1234}$: 37 diagrams							
i	11	222	3333	44444			
j	01	012	0123	01234			
#	M_{ij}				$(S,D,T;N)$	M	W^{-1}
13.2.4, 13.3.5	00	011	1210	31000	(1,1,0;6)	7962624	24
12.3.1, 12.4.4	00	011	1300	30100	(1,0,1;6)	2654208	72
11.4.5, 15.3.1, 15.4.1	00	011	2110	22000	(1,1,0;4)	11943936	16
11.1.3, 11.2.1	00	020	1120	31000	(0,2,0;6)	7962624	24
8.1.1, 17.1.1	00	020	2020	22000	(0,3,0;8)	2985984	64
9.1.1, 13.2.1	00	020	2110	21100	(0,1,0;16)	5971968	32
15.2.3, 15.4.6	00	021	1101	31000	(2,1,0;6)	3981312	48
17.1.4, 17.2.4	00	021	1200	30010	(1,2,0;6)	3981312	48
14.1.4, 15.4.4	00	021	2100	21010	(1,1,0;8)	5971968	32
12.2.1, 12.4.2	00	030	1011	31000	(1,0,1;6)	2654208	72

(Table 13.7 continued.)

$\mathbf{G}^{\mathrm{c},(4)}_{1234}$: 37 diagrams							
i	11	222	3333	44444			
j	01	012	0123	01234			
#	M_{ij}				$(S,D,T;N)$	M	W^{-1}
14.3.1, 14.4.1	00	030	1110	30010	(0,0,1;12)	2654208	72
10.2.2, 12.4.1	00	030	2010	21010	(0,0,1;8)	3981312	48
11.2.4, 11.3.2, 17.1.2, 17.2.1	00	101	1210	22000	(1,2,0;2)	11943936	16
12.3.2, 12.4.3, 14.2.2, 14.3.2	00	101	1300	21100	(1,0,1;2)	7962624	24
9.2.2, 14.1.1, 14.4.3	00	110	1120	22000	(0,2,0;4)	11943936	16
9.1.3, 9.2.3, 11.1.1, 11.4.1	00	110	1210	21100	(0,1,0;2)	47775744	4
10.1.1, 10.2.3, 14.2.1, 14.4.2	00	110	1300	20200	(0,1,1;2)	7962624	24
13.3.2, 15.2.1, 15.3.3	00	111	1101	22000	(2,1,0;4)	5971968	32
11.2.3, 11.4.2, 13.2.2, 13.3.1	00	111	1200	21010	(1,1,0;2)	23887872	8
8.1.3, 11.1.2, 11.3.1	00	120	1200	20110	(0,2,0;4)	11943936	16
15.1.4, 15.4.5	01	001	1120	31000	(2,1,0;6)	3981312	48
13.1.3, 16.1.1	01	001	2110	21100	(2,0,0;16)	2985984	64
16.1.4, 16.2.1	01	011	1011	31000	(3,0,0;6)	3981312	48
15.3.4, 15.5.4	01	011	1110	30010	(2,0,0;12)	3981312	48
12.1.3, 16.1.2	01	011	2010	21010	(2,0,0;8)	5971968	32
11.3.3, 11.4.4, 12.1.1, 12.4.5	01	100	1120	21100	(1,1,0;2)	23887872	8
14.1.3, 14.2.3, 17.1.3, 17.3.1	01	100	1210	20200	(1,2,0;2)	11943936	16
15.1.2, 15.5.3, 16.1.3, 16.2.2	01	101	1101	21100	(3,0,0;2)	11943936	16
13.1.2, 13.3.4, 15.4.2, 15.5.1	01	101	1110	21010	(2,0,0;2)	23887872	8
15.1.3, 15.4.3, 17.2.3, 17.3.2	01	101	1200	20110	(2,1,0;2)	11943936	16
12.1.4, 12.3.3, 15.1.1, 15.3.2	01	110	1101	20200	(2,1,0;2)	11943936	16
11.4.6, 13.1.1, 13.2.3	01	110	1110	20110	(1,0,0;4)	23887872	8
8.1.2, 9.2.1, 10.2.1	10	100	1120	12100	(0,2,0;4)	11943936	16
12.1.2, 12.2.2, 13.3.3, 17.2.2	10	101	1101	12100	(2,1,0;2)	11943936	16
11.2.2, 11.4.3, 14.1.2, 14.3.3	10	101	1110	12010	(1,1,0;2)	23887872	8
9.1.2	10	110	1110	11110	(0,0,0;24)	7962624	24
15.2.2, 15.5.2	10	111	1101	11001	(3,0,0;6)	3981312	48

14

Path Integral Calculation of Effective Action. Loop Expansion

The path integral formula for $Z[j]$ can be employed for a direct to evaluation of the effective action of a theory. Diagrammatically, the result will be the loop expansion organized by powers of the Planck quantum $\hbar$.

14.1 General Formalism

Consider the generating functional of all Green functions

$$Z[j] = e^{iW[j]/\hbar}, \tag{14.1}$$

where $W[j]$ is the generating functional of all *connected* Green functions. The vacuum expectation of the field, the average

$$\Phi(x) \equiv \langle \phi(x) \rangle, \tag{14.2}$$

is given by the first functional derivative

$$\Phi(x) = \delta W[j]/\delta j(x). \tag{14.3}$$

This can be inverted to yield $j(x)$ as an x-dependent functional of $\Phi(x)$:

$$j(x) = j[\Phi](x). \tag{14.4}$$

This is used to form the Legendre transform of $W[j]$:

$$\Gamma[\Phi] \equiv W[j] - \int d^4x j(x)\Phi(x). \tag{14.5}$$

where the right-hand side is replaced by (14.5) This is the *effective action* of the theory. Its first functional derivative gives back the current

$$\frac{\delta\Gamma[\Phi]}{\delta\Phi(x)} = -j(x). \tag{14.6}$$

The generating functional of all connected Green functions can be recovered from the effective action by the inverse Legendre transform

$$W[j] = \Gamma[\Phi] + \int d^4x j(x)\Phi(x). \tag{14.7}$$

Let us compare this with the the path integral formula for the generating functional $Z[j]$:

$$Z[j] = \frac{\int \mathcal{D}\phi(x) e^{(i/\hbar)\left\{\mathcal{A}[\phi]+\int d^4x j(x)\phi(x)\right\}}}{\int \mathcal{D}\phi(x) e^{(i/\hbar)\mathcal{A}_0[\phi]}}. \tag{14.8}$$

With (14.1), this amounts to the path integral formula for $\Gamma[\Phi]$:

$$e^{\frac{i}{\hbar}\left\{\Gamma[\Phi]+\int d^4x j(x)\Phi(x)\right\}} = N\int \mathcal{D}\phi(x) e^{(i/\hbar)\left\{\mathcal{A}[\phi]+\int d^4x j(x)\phi(x)\right\}} \tag{14.9}$$

with the normalization factor

$$\mathcal{N} = \left\{\int \mathcal{D}\phi(x) e^{(i/\hbar)\mathcal{A}_0[\phi]}\right\}^{-1}. \tag{14.10}$$

In writing this we have explicitly displayed the action quantum $\hbar$, which is a measure for the size of quantum fluctuations. There are many physical systems, for which quantum fluctuations are rather small except in the immediate vicinity of certain critical points. For these systems, it is desirable to develop a method of evaluating (14.9) as an expansion in powers of $\hbar$, which amounts to taking into account successively increasing quantum fluctuations.

For $\hbar \to 0$, the path integral over the field $\phi(x)$ in (14.8) is dominated by the classical solution $\phi_{\rm cl}(x)$ which extremizes the exponent

$$\left.\frac{\delta\mathcal{A}}{\partial\phi}\right|_{\phi=\phi_{\rm cl}(x)} = -j(x). \tag{14.11}$$

At this level we therefore can identify

$$W[j] = \Gamma[\Phi] + \int d^4x j(x)\Phi(x) \quad = \quad \mathcal{A}[\phi_{\rm cl}] + \int d^4x j(x)\phi_{\rm cl}(x). \tag{14.12}$$

Of course, $\phi_{\rm cl}(x)$ is a functional of $j(x)$, so that we may write it more explicitly, as $\phi_{\rm cl}[j](x)$. By differentiating $W[j]$ with respect to j, we have from the general fist part of Eq. (14.2):

$$\Phi(x) = \frac{\delta W}{\delta j} = \frac{\delta\Gamma}{\delta\Phi}\frac{\delta\Phi}{\delta j} + \Phi + j\frac{\delta\Phi}{\delta j}. \tag{14.13}$$

Inserting the classical field equation (14.11), this becomes

$$\Phi(x) = \frac{\delta\mathcal{A}}{\delta\phi_{\rm cl}}\frac{\delta\phi_{\rm cl}}{\delta j} + \phi_{\rm cl} + j\frac{\delta\phi_{\rm cl}}{\delta j} = \phi_{\rm cl}. \tag{14.14}$$

Thus, to this approximation, $\Phi(x)$ coincides with the classical field $\phi_{\rm cl}(x)$. Replacing $\phi_{\rm cl}(x) \to \Phi(x)$ on the right-hand side of Eq. (14.12), we therefore obtain the lowest-order result (zeroth order in $\hbar$):

$$\Gamma[\Phi] = \mathcal{A}[\Phi] \tag{14.15}$$

i.e., the effective action equals the fundamental action.

We have shown in Chapter 12 that all vertex functions can be obtained from the derivatives of $\Gamma[\Phi]$ with respect to Φ at the equilibrium value of Φ for $j = 0$. For the ϕ^4-theory with O(N)-symmetry the zeroth-order effective action is

$$\Gamma[\Phi] = \int d^4x \left[\frac{1}{2}\left(\partial\Phi_a\right)^2 - \frac{m^2}{2}\Phi_a^2 - \frac{g}{4!}\left(\Phi_a^2\right)^2\right]. \tag{14.16}$$

For massive particles,[1] this has an extremum at $\Phi \equiv 0$, and there are only two non-vanishing vertex functions $\Gamma^{(n)}(x_1, \dots, x_n)$:

***n*=2**

$$\begin{aligned}\Gamma^{(2)}(x_1, x_2)_{ab} &\equiv \left.\frac{\delta^2\Gamma}{\delta\Phi_a(x_1)\delta\Phi_b(x_2)}\right|_{\Phi_a=0} = \left.\frac{\delta^2\mathcal{A}}{\phi_a(x_1)\phi_b(x_2)}\right|_{\phi_a=\Phi_a=0}\\ &= (-\partial^2 - m^2)\delta_{ab}\delta^{(4)}(x_1 - x_2).\end{aligned} \tag{14.17}$$

This determines the inverse of the propagator:

$$\Gamma^{(2)}(x_1, x_2)_{ab} = [iG^{-1}]_{ab}(x_1, x_2), \tag{14.18}$$

Thus we find to this zeroth-order approximation that $G_{ab}(x_1, x_2)$ is equal to the free propagator:

$$G_{ab}(x_1, x_2) = G_{0ab}(x_1, x_2) \tag{14.19}$$

***n*=4**

$$\Gamma^{(4)}(x_1, x_2, x_3, x_4)_{abcd} \equiv \frac{\delta^4\Gamma}{\delta\Phi_a(x_1)\delta\Phi_b(x_2)\delta\Phi_c(x_3)\delta\Phi_d(x_4)} = gT_{abcd}, \tag{14.20}$$

with

$$(!!)^4T_{abcd} = \frac{1}{3}(\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}), \tag{14.21}$$

which is just the fundamental vertex (9.223).

According to the definition of the effective action, all diagrams of the theory can be composed from the propagator $G_{ab}(x_1, x_2)$ and this vertex via tree diagrams. Thus we see that in this lowest approximation, we recover precisely the subset of all original Feynman diagrams with a tree-like topology. These are all diagrams which do not involve any loop integration. Since the limit $\hbar \to 0$ corresponds to the classical equations of motion with no quantum fluctuations we conclude: Classical field theory corresponds to tree diagrams.

The use of the initial action as an approximation to the effective action neglecting fluctuations is often referred to as mean-field theory.

---

[1] Also the case $m^2 < 0$ corresponds to physical systems and will be discussed separately

14.2 Quadratic Fluctuations

In order to find the $\hbar$-correction to this approximation we expand the action in powers of the fluctuations of the field around the classical solution

$$\delta\phi(x) \equiv \phi(x) - \phi_{\rm cl}(x), \tag{14.22}$$

and perform a perturbation expansion. The quadratic term in $\delta\phi(x)$ is taken to be the free-field action, the higher powers in $\delta\phi(x)$ are the interactions. Up to second order in the fluctuations $\delta\phi(x)$, the action is expanded as follows:

$$\begin{aligned} &\mathcal{A}[\phi_{\rm cl} + \delta\phi] + \int d^4x j(x)[\phi_{\rm cl}(x) + \delta\phi(x)] \\ &\quad = \mathcal{A}[\phi_{\rm cl}] + \int d^4x j(x)\phi_{\rm cl}(x) + \int d^4x \left\{ j(x) + \left.\frac{\delta\mathcal{A}}{\delta\phi(x)}\right|_{\phi=\phi_{\rm cl}} \right\} \delta\phi(x) \\ &\quad + \int d^4x d^4y \; \delta\phi(x) \left.\frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)}\right|_{\phi=\phi_{\rm cl}} \delta\phi(y) + \mathcal{O}\left((\delta\phi)^3\right). \end{aligned} \tag{14.23}$$

The curly bracket multiplying the linear terms in the variation $\delta\Phi$ vanish due to the extremality property of the classical field $\phi_{\rm cl}$ expreesed by the field equation (14.11). Inserting this expansion into (14.9), we obtain the approximate expression

$$Z[j] \approx \mathcal{N} e^{(i/\hbar)\left\{\mathcal{A}[\phi_{\rm cl}]+\int d^4xj\phi_{\rm cl}\right\}} \int \mathcal{D}\delta\phi \exp\left\{ \frac{i}{\hbar} \int d^4x d^4y \; \delta\phi(x) \left.\frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)}\right|_{\phi=\phi_{\rm cl}} \delta\phi(y) \right\} \tag{14.24}$$

We now observe that the fluctuations in $\delta\phi$ will be of average size $\sqrt{\hbar}$ due to the $\hbar$-denominator in the Fresnel integrals over $\delta\phi$ in (14.24). Thus the fluctuations $(\delta\phi)^n$ are on the average of relative order $\hbar^{n/2}$. If we ignore corrections of order $\hbar^{3/2}$, the fluctuations remain quadratic in $\delta\phi$ and we may calculate the right-hand side of (14.24) as

$$\begin{aligned} &\mathcal{N} e^{(i/\hbar)\left\{\mathcal{A}[\phi_{\rm cl}]+\int d^4xj(x)\phi_{\rm cl}(x)\right\}} \left[\det \frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)}\right]_{\phi=\phi_{\rm cl}} \\ &\quad = \left(\det iG_0\right)^{1/2} e^{(i/\hbar)\left\{\mathcal{A}[\phi_{d}]+\int d^4xj(x)\phi_{\rm cl}(x)+i\frac{\hbar}{2}{\rm Tr}\log[\delta^2\mathcal{A}/\delta\phi(x)\delta\phi(y)|_{\phi=\phi_{\rm cl}}\right\}}. \end{aligned} \tag{14.25}$$

Comparing this with the left-hand side of (14.9), we find that to first order in $\hbar$, the effective action may be recovered by equating

$$\Gamma[\Phi] + \int d^4x j(x)\Phi(x) = \mathcal{A}[\phi_{\rm cl}] + \int d^4x j\phi_{\rm cl} + \frac{i\hbar}{2}{\rm Tr}\,\log\frac{\delta^2\mathcal{A}}{\delta\phi(x)\delta\phi(y)}\,(\phi_{\rm cl}). \tag{14.26}$$

In the limit $\hbar \to 0$, the trace log term disappears and (14.26) reduces to the classical action.

To include the $\hbar$-correction into $\Gamma[\Phi]$, we expand $W[j]$ as

$$W[j] = W_0[j] + \hbar W_1[j] + \mathcal{O}(\hbar^2). \tag{14.27}$$

Correspondingly, the field Φ differs from $\Phi_{\rm cl}$ by a correction of order $\hbar^2$.

$$\Phi = \phi_{\rm cl} + \hbar\phi_1 + \mathcal{O}(\hbar^2). \tag{14.28}$$

Inserting this into (14.26), we find

$$\begin{aligned}\Gamma[\Phi] + \int d^4x j\Phi \;&=\; \mathcal{A}\left[\Phi - \hbar\phi_1\right] + \int d^4x j\Phi - \hbar \int d^4x j\phi_1 + \frac{i}{2}\hbar \mathrm{Tr}\,\log \left.\frac{\delta^2 \mathcal{A}}{\delta\phi_a\delta\phi_b}\right|_{\phi=\Phi-\hbar\phi_1}\\ &\quad +\mathcal{O}\left(\hbar^2\right).\end{aligned}$$

Expanding the action up to the same order in $\hbar$ gives

$$\begin{aligned}\Gamma[\Phi] \;&=\; \mathcal{A}[\Phi] + \hbar\left\{\frac{\delta\mathcal{A}[\Phi]}{\delta\Phi} - j\right\}\phi_1 + \int d^4x\, j\Phi + \frac{i}{2}\hbar \mathrm{Tr}\,\log \left.\frac{\delta^2\mathcal{A}}{\delta\phi_a\delta\phi_b}\right|_{\phi=\Phi}\\ &\quad +\mathcal{O}\left(\hbar^2\right).\end{aligned} \tag{14.29}$$

But because of (14.11), the curly-bracket term is only of order $\mathcal{O}(\hbar^2)$, so that we find the one-loop form of the effective action

$$\begin{aligned}\Gamma[\Phi] = \Gamma_0[\Phi] + \Gamma_1[\Phi] \;&=\; \int d^4x \left[\frac{1}{2}\left(\partial\Phi\right)^2 - \frac{m^2}{2}\Phi_a^2 - \frac{g}{4!}\left(\phi_a^2\right)^2\right]\\ &\quad +\frac{i}{2}\hbar \mathrm{Tr}\,\log\left[-\partial^2 - m^2 - \frac{g}{6}\left(\delta_{ab}\Phi_c^2 + 2\Phi_a\Phi_b\right)\right].\end{aligned} \tag{14.30}$$

In the special case of a one-component real field, this becomes

$$\Gamma[\Phi] = \int d^4x \left[\frac{1}{2}(\partial\Phi)^2 - \frac{m^2}{2}\Phi^2 - \frac{g}{4!}\Phi^4\right] + . \tag{14.31}$$

What is the graphical content of the set of all Green functions at this level? For $j = 0$, we find that the minimum lies at $\Phi = \Phi^0 \equiv \Phi_j = 0$, as in the mean-field approximation. Around this minimum, we may expand the trace log in powers of Φ, and obtain

$$\begin{aligned}\frac{i}{2}\hbar\mathrm{Tr}\log\left(-\partial^2-m^2-\frac{g}{2}\Phi^2\right) &= \frac{i}{2}\hbar\mathrm{Tr}\log\left(-\partial^2-m^2\right) + \frac{i}{2}\hbar\mathrm{Tr}\log\left(1+\frac{i}{-\partial^2-m^2}ig\frac{\Phi^2}{2}\right)\\ &= i\frac{\hbar}{2}\mathrm{Tr}\log\left(-\partial^2 - m^2\right) - i\frac{\hbar}{2}\sum_{n=1}^{\infty}\left(-i\frac{g}{2}\right)^n \frac{1}{n}\mathrm{Tr}\left(\frac{i}{-\partial^2-m^2}\Phi^2\right)^n.\end{aligned} \tag{14.32}$$

If we insert

$$G_0 = \frac{i}{-\partial^2 - m^2}, \tag{14.33}$$

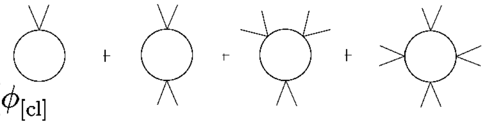
this can be written as

$$i\frac{\hbar}{2}\mathrm{Tr}\,\log\left(-\partial^2 - m^2\right) - i\frac{\hbar}{2}\sum_{n=1}^{\infty}\left(-i\frac{g}{2}\right)^n\frac{1}{n}\mathrm{Tr}\,\left(G_0\Phi^2\right)^n. \tag{14.34}$$

More explicitly, the terms with $n = 1$ and $n = 2$ read:

$$
\begin{aligned}
&-\frac{\hbar}{2} g \int d^4x d^4y \delta^{(4)}(x-y) G_0(x,y) \Phi^2(y) \\
&+i\hbar \frac{g^2}{16} \int d^4x d^4y d^4z \delta^4(x-z) G_0(x,y) \Phi^2(y) G_0(y,z) \Phi^2(z) + \dots \quad . \qquad (14.35)
\end{aligned}
$$

The expansion terms of (14.34) for $n \geq 1$ correspond obviously to the Feynman diagrams



$\mathcal{A}[\phi_{[cl]}$ (14.36)

Thus the series (14.34), is a sum of all diagrams with one loop and any number of fundamental Φ^4 vertices

To systematize the entire expansion (14.34), the trace log term may be pictured by a single-loop diagram

$$
i\frac{\hbar}{2} \mathrm{Tr} \log \left(-\partial^2 - m^2 \right) = \bigcirc \quad . \qquad (14.37)
$$

The first two diagrams in (14.36) contribute corrections to the vertices $\Gamma^{(2)}$ and $\Gamma^{(4)}$ of (14.17), (14.20). The remaining ones produce higher vertex functions and lead to more involved tree diagrams. Note that only the first two corrections are formally divergent, all other Feynman integrals converge. In momentum space we find from (14.35)

$$
\begin{aligned}
\Gamma^{(2)}(q) &= q^2 - m^2 - \hbar \frac{g}{2} \int \frac{dk^4}{(2\pi)^4} \frac{i}{k^2 - m^2 + i\eta} && (14.38) \\
\Gamma^{(4)}(q_i) &= g - i\frac{g^2}{2} \left[\int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2 - m^2 + i\epsilon} \frac{i}{(q_1 + q_2 - k)^2 - m^2 + i\eta} + 2 \text{ perm} \right] . \\
& && (14.39)
\end{aligned}
$$

The convergence of all higher diagrams the expansion (14.36) is a reflection of the renormalizability of the theory since only up to $n = 4$ does one have the possibility to add counter terms of the same form as the original Lagrangian. We may write (14.38) in euclidean form as

$$
\begin{aligned}
\Gamma^{(2)}(q) &= -q^2 - m^2 - \hbar \frac{g}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2} \\
&= -\left(q^2 + m^2 + \hbar \frac{g}{2} D_1 \right), && (14.40) \\
\Gamma^{(4)}(q_i) &= g - \hbar \frac{g^2}{2} \left[I\left(q_1 + q_2\right) + 2 \text{ perm} \right]. && (14.41)
\end{aligned}
$$

These are renormalized with the help of counter terms calculated in Section 9.3, yielding the renormalized diagrams

$$\begin{aligned}\Gamma_R^{(2)}(q) &= -(q^2+m^2), &(14.42)\\ \Gamma_R^{(4)}(q_i) &= g-\hbar\frac{g^2}{2}\left\{\left[I\left(q_1+q_2\right)+2 \text{ perm}\right]-3I(0)\right\}. &(14.43)\end{aligned}$$

If we regularize the integrals dimensionally in $4-\epsilon$ dimensions, the counterterms take the forms calculated in Section 9.5, and (14.42) becomes

$$\begin{aligned}\Gamma_R^{(2)}(q) &= -\left\{q^2+m^2+\hbar\frac{g}{2}S_D\mu^{-\epsilon}m^2\right.\\ &\qquad\left.\times\left[\frac{1}{2}\Gamma(2-\epsilon/2)\Gamma\left(-1+\epsilon/2\right)\left(\frac{m^2}{\mu^2}\right)^{-\epsilon/c}+\frac{1}{\epsilon}\right]\right\}, &(14.44)\\ \Gamma_R^{(4)}(q_i) &= g-\hbar\frac{g^2}{2}\left[I_R\left(q_1+q_2\right)+2 \text{ perm}\right]. &(14.45)\end{aligned}$$

where [compare (9.173)]

$$I_R(q)=-\frac{1}{2}S_D\mu^{-\epsilon}\left[1+L^m(q)+\log\frac{q^2}{\mu^2}\right]+\mathcal{O}(\epsilon). \tag{14.46}$$

As far as the original effective action (14.31) to order $\hbar$ is concerned, we may add the counter terms as

$$\begin{aligned}\Gamma[\Phi] &= \int d^4x\left\{\frac{1}{2}(\partial\Phi)^2-\frac{m^2}{2}\Phi^2-\frac{g}{4!}\Phi^4\right\}-i\frac{\hbar}{2}\text{Tr}\log\left(-\partial^2-m^2-\frac{g}{2}\Phi^2\right)\\ &\quad+\frac{g}{4}\int\frac{d^4q}{(2\pi)^4}\frac{1}{q^2+m^2}\int d^4x\,\Phi^2(x)-\frac{g^2}{16}\int\frac{d^4q}{(2\pi)^4}\frac{1}{\left(q^2+m^2\right)}\int d^4x\,\Phi^4\end{aligned}$$

The divergent integrals in the last two terms can be evaluated with any regularization method. In dimensional regularization in $4-\epsilon$ dimensions, only the singular $1/\epsilon$-parts of the two integrals are selected, and (14.47) becomes

$$\begin{aligned}\Gamma[\Phi] &= \int d^4x\left\{\frac{1}{2}(\partial\Phi)^2-\frac{m^2}{2}\Phi^2-\frac{g}{4!}\Phi^4\right\}+i\frac{\hbar}{2}\text{Tr}\log\left(-\partial^2-m^2-\frac{g}{2}\Phi^2\right)\\ &\qquad-{}^mC\frac{m^2}{2}\Phi^2-{}^gC_1\frac{g^2}{4!}\Phi^4. &(14.47)\end{aligned}$$

The expansions in powers of ϵ has an interesting feature which is worth pointing out at this place and which has interesting applications in the description of critical phenomena. For small g, Eq. (14.44) can be rewritten as

$$\Gamma_R^{(2)}=-\left(q^2+m^2+\hbar\frac{g}{4}S_D\log\frac{m^2}{\mu^2}\right) \tag{14.48}$$

which is, to the same order in g, equal to

$$\Gamma_R^{(2)}(q) = -\left[q^2 + \left(\frac{m^2}{\mu^2}\right)^{1+\hbar\frac{g}{4}\bar{S}_D} \mu^2\right]. \tag{14.49}$$

This means that the vertex function at $q = 0$ has a non-integer power in the mass parameter which depends on the coupling strength.

$$\Gamma_R^{(2)}(0) = -\left(\frac{m^2}{\mu^2}\right)^{\gamma} \mu^2 \tag{14.50}$$

where

$$\gamma = 1 + \hbar\frac{g}{4}\bar{S}_D \tag{14.51}$$

The important point is that this power γ is measureable as an experimental quantity called the *susceptibility*. It is the so-called *critical exponent* of the susceptibility [see (21.153).[2] A similar power behaviour is found for $\Gamma^{(4)}$, but here only in the limit $m^2 \to 0$ where $L^m \sim \log m^2/\mu^2$, and thus

$$\begin{aligned} \Gamma^{(4)} \quad & \underset{m\to 0}{\longrightarrow} \quad g\left(1 + \hbar\frac{3}{4}g\bar{S}_D \log\frac{m^2}{\mu^2}\right) + \mathcal{O}(m^2) \\ & = \quad g\left(\frac{m^2}{\mu^2}\right)^{\hbar\frac{3}{4}g\bar{S}_D} . \end{aligned} \tag{14.52}$$

Also this power behaviour is measurable and defines the critical index β via the so-called scaling relation

$$\gamma - \beta \equiv 1 + \hbar\frac{3}{4}g\bar{S}_D. \tag{14.53}$$

The higher powers of Φ are accompanied by terms which are more and more singular in the limit $m \to 0$. We see from the Feynman integrals in (14.34) that the diagrams in (14.36) diverge like $m^{4-\epsilon-n}$ for the effective action terms Φ^n.

14.3 Massless Theory

The case $m = 0$ deserves special attention. It is often referred to the *critical theory*. This name reflects the relevance of this limit for the behaviour of physical systems at a critical temperature where fluctuations are of infinite range. Let us study directly the effective potential of a critical ϕ^4-theory at a constant field Φ at the one loop level. It is defined by $v(\Phi) = -\Gamma[\Phi]/VT$. Then the argument in the trace log term becomes diagonal in momentum space and reduces to a simple momentum integral.

---

[2] In Section 21.8 we shall see that the coupling strength governing the behavior of all observable quantities in the limit $m^2 \to 0$ is given by $\left(\hbar g\bar{S}_D = \frac{2}{3}\epsilon\right)$.

After a Wick rotation the trace log term, it can be calculated, and the renormalized potential corresponding to the effective action (14.47) can be written as

$$\begin{aligned} v(\Phi) &= \frac{m^2}{2}\Phi^2 + \frac{g}{4!}\Phi^4 + \frac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\log\left(1+\frac{g}{2}\frac{\Phi^2}{q^2+m^2}\right) \\ &\quad - \frac{g}{4}\int \frac{d^Dq}{(2\pi)^D}\frac{1}{q^2+m^2}\Phi^2 + \frac{g^2}{16}\int \frac{d^Dq}{(2\pi)^D}\frac{1}{\left(q^2+m^2\right)^2}\Phi^4, \end{aligned} \tag{14.54}$$

where we dropped the infinite additive constant

$$\frac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\log\left(q^2+m^2\right).$$

If we attempt to take this expression to the $m = 0$-limit, the counter terms are no longer defined. We now see an important advantage of the ϵ-expansion: The singular $1/\epsilon$-terms are independent of the mass, so that the poles at $\epsilon = 0$

$$-\frac{q\mu^{-\epsilon}}{4}m^2\tilde{S}_D\left(-\frac{1}{\epsilon}\right)\Phi^2, \quad \frac{g_R^{2-\epsilon}}{16}\tilde{S}_D\frac{1}{\epsilon}\Phi^4 \tag{14.55}$$

regularize the potential for any mass. Note, however, that an auxiliary mass μ had to be introduced to define these expressions. In the case $m \neq 0$, μ can be chosen equal to m. But for $m = 0$ we must use an arbitrary nonzero auxiliary mass.

Let us now check that the effective potential remains indeed finite for $m = 0$. There, $v(\Phi)$ becomes

$$v(\Phi) = \frac{g}{4!}\Phi^4 + \frac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\log\left(1+\frac{q}{2}\frac{\Phi^2}{q^2}\right) + \frac{g}{16}\mu^{-\epsilon}\frac{1}{\epsilon}\Phi^4. \tag{14.56}$$

and displays an important feature: When expanding the logarithm in powers of Φ, the expansion terms correspond to increasingly divergent Feynman integrals

$$\int \frac{d^Dq}{(2\pi)^D}\frac{1}{(q^2)^n}.$$

Contrary to the previously regularized divergencies coming from the large-q^2 regime, these divergencies are due to the $q = 0$ -singularity of the massless propagators $G_0(q) = i/q^2$. Such infrared (IR) divergences were encountered before in quantum electrodynamics in Chapter 10. It is a pleasant feature of the sum over all one loop diagrams that the final result has lost these IR singularities in favor of a weak logarithmic singularity which is integrable then by removing the IR problem. The only singularities which remain are the is the ultraviolet one which is taken care of by the counter term.

Let us calculate the renormalized potential explicitly. For this we have to extend the formulas of dimensional regularization to the integral in (14.56). Using

$$\int d^Dk\frac{1}{\left(k^2+m^2\right)} = \tilde{S}_D\frac{1}{2}\frac{\Gamma(D/2)\Gamma(1-D/2)}{\Gamma(1)}\frac{1}{\left(m^2\right)^{1-D/2}} \tag{14.57}$$

we integrate in m^2 and find

$$\int \bar{d}^D k \log\left(k^2+m^2\right) = \bar{S}_D \frac{1}{2} \frac{\Gamma(D/2)\Gamma(1-D/2)}{\Gamma(1)} \frac{2}{D} \left(m^2\right)^{D/2}. \tag{14.58}$$

In $4-\epsilon$ dimensions, this behaves like

$$\bar{S}_D \left[-1/\epsilon + \mathcal{O}(\epsilon)\right] \frac{1}{2} (1+\epsilon) \left(m^2\right)^{\frac{2-\epsilon}{2}}, \tag{14.59}$$

So that the potential becomes

$$v(\Phi) \;=\; \frac{g}{4!}\Phi^4 + \frac{1}{4}\bar{S}_D \left(-\frac{1}{\epsilon}-\frac{1}{4}\right)\left(\frac{g}{2}\Phi^2\right)^{2-\frac{\epsilon}{2}} + \frac{g^2}{16}\bar{S}_D \mu^{-\epsilon}\frac{1}{\epsilon}\Phi^4. \tag{14.60}$$

To perform an ϵ-expansion of this log, we divide the coupling constant and field by a scale parameter avoiding μ. Then $g\mu^{-\epsilon}, \Phi/\mu^{1-(\epsilon/2)}$ are dimensionless quantities in terms of which

$$\begin{aligned} v(\Phi) \;&=\; \mu^{4-\epsilon}\left[\frac{g\mu^{-\epsilon}}{4!}\left(\frac{\Phi}{\mu^{\epsilon-1/2}}\right)^4 + \frac{1}{4}\bar{S}_D\left(-\frac{1}{\epsilon}-\frac{1}{4}\right)\left(\frac{g\mu^{-\epsilon}}{2}\frac{\Phi^2}{\mu^{2-\epsilon}}\right)^{2-\frac{\epsilon}{2}}\right] \\ &\quad + \frac{g^2}{16}\frac{\mu^{-2\epsilon}}{\epsilon}\bar{S}_D\left(\frac{\Phi}{\mu^{1-\epsilon/2}}\right)^4. \end{aligned} \tag{14.61}$$

If we use the dimensionless coupling constant $\lambda \equiv \bar{S}_D g\mu^{-\epsilon}$ and the field $\tilde{\Phi}) = \Phi/\mu^{1-\epsilon/2}$ as new variables

$$v(\Phi) = \frac{\mu^{4-\epsilon}}{\bar{S}_D}\left[\frac{\lambda}{4!}\tilde{\Phi}^4 + \frac{1}{4}\left(-\frac{1}{\epsilon}-\frac{1}{4}\right)\left(\frac{\lambda\tilde{\Phi}^2}{2}\right)^2\left(1-\frac{\epsilon}{2}\log\frac{\lambda\tilde{\Phi}^2}{2}\right) + \frac{\lambda^2\tilde{\Phi}^4}{16\epsilon}\tilde{\Phi}^4\right\}. \tag{14.62}$$

The prefactor is equal to $\mu^4 8\pi^2$ to zeroth order in ϵ. Thus the massless limit of the effective potential is well defined in 4 dimensions. There is, however, a special feature: The expression has become finite at the loss of introducing the extra parameter μ.

Another important property of the critical potential is that it can no longer be expanded in a power series in Φ. Instead, we may rewrite the expression correctly up to order λ^2 as

$$\begin{aligned} v(\Phi) \;&=\; \frac{\mu^{4-\epsilon}}{\bar{S}_D}\frac{1}{6}\left\{\left[\frac{\lambda}{2}\left(1-\frac{3}{16}\lambda\right)\tilde{\Phi}^2\right]^2 + \frac{3}{8}\left(\frac{\lambda}{2}\tilde{\Phi}^2\right)^2\log\frac{\lambda}{2}\tilde{\Phi}^2\right\} \\ &=\; \frac{\mu^{4-\epsilon}}{\bar{S}_D}\frac{1}{6\lambda}\left[\frac{\lambda}{2}\left(1-\frac{3}{16}\lambda\right)\tilde{\Phi}^2\right]^{2+\frac{3}{4}\lambda} + \mathcal{O}(\lambda^3). \end{aligned} \tag{14.63}$$

Such a non-integer power behaviour is observed in critical systems. The power of $\tilde{\Phi}^2$ is referred to as critical index $1+\delta$, so that here $\delta = 3+\frac{3}{2}\lambda$.

It should be pointed out that the potential in the first line of (14.63) has another minimum away from the origin at

$$\frac{\lambda}{3!}\tilde{\Phi}^3 + \frac{\lambda^2}{8}\tilde{\Phi}^3\left(\log\frac{\lambda}{2}\tilde{\Phi}^2 - \frac{1}{2}\right) + \frac{\lambda^2}{16}\tilde{\Phi}^3 = 0. \tag{14.64}$$

This is solved by

$$\lambda\,\log\frac{\lambda}{2}\tilde{\Phi}^2 = -\frac{4}{3} \tag{14.65}$$

or

$$\tilde{\Phi}^2 = \frac{2}{\lambda}e^{-4}3\lambda. \tag{14.66}$$

However such a solution found for small λ cannot be trusted. The higher loops to be discussed later and neglected up to this point will produce more powers of $\lambda\log\lambda\tilde{\Phi}^2/2$, and the series cannot be expected to converge at such a large λ. As a matter of fact, the approximate exponentiation performed in the second line of (14.63) does not show this minimum and will be seen, via the methods to be described later, to be the correct analytic form of the potential to all orders in λ for small enough ϵ and λ.

14.4 Effective Action to Order $\hbar^2$

Let us now find the next correction to the effective action.[3] Instead of truncating the expansion (14.23), we keep all terms, reorganizing only the linear and quadratic terms as in the passage to (14.24). This yields the exact expression

$$e^{\frac{i}{\hbar}\{\Gamma[\Phi]+j\Phi\}} = e^{\frac{i}{\hbar}W[j]} = e^{\frac{i}{\hbar}(\mathcal{A}[\phi_{\rm cl}]+j\phi_{\rm cl})-\frac{\hbar}{2}{\rm Tr}\log\mathcal{A}_{\phi\phi}[\phi_{\rm cl}]}e^{\frac{i}{\hbar}\hbar^2W_2[\phi_{\rm cl}]} \tag{14.67}$$

where $W_2[\phi_{\rm cl}]$ is defined by

$$e^{\frac{i}{\hbar}\hbar^2W_2[\phi_{\rm cl}]} = \frac{\int\mathcal{D}\phi e^{\frac{i}{\hbar}\left\{\frac{1}{2}\phi\mathcal{A}_{\phi\phi}[\phi_{\rm cl}]\phi+I[\phi_{\rm cl},\phi]\right\}}}{\int\mathcal{D}\phi e^{\frac{i}{\hbar}\left\{\frac{1}{2}\phi\mathcal{A}_{\phi\phi}[\phi_{\rm cl}]\phi\right\}}}, \tag{14.68}$$

and I is the remainder of the fluctuating action

$$I\left[\phi_{\rm cl},\phi\right] = \mathcal{A}\left[\phi_{\rm cl}+\phi\right] - \mathcal{A}[\phi_{\rm cl}] - \frac{1}{2}\phi\mathcal{A}_{\phi\phi}[\phi_{\rm cl}]\phi. \tag{14.69}$$

The subscript ϕ denotes functional differentiation and integration symbols. Adjacent space-time variables have been omitted, for brevity. We have renamed $\delta\phi(x)$ by $\phi(x)$.

Note that by construction, I is at least cubic in ϕ. Thus the path integral (14.69) may be considered as the generating functional Z of a theory of ϕ field with a propagator

$$\mathcal{D}[\Phi_{\rm cl}] = i\mathcal{A}_{\phi\phi}[\phi_{\rm cl}]^{-1}$$

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[3] R. Jackiw, Phys. Rev. D *9*, 1687 (1976)

and an interaction I which both depend in a complicated manner on j via $\phi_{\rm cl}$. We know from the previous sections, and will immediately see this explicitly, that $\hbar^2 W_2$ is indeed of order $\hbar^2$. Let us again set

$$\phi = \phi_{\rm cl} + \hbar\phi_1. \tag{14.70}$$

We shall express $W[j]$ in the form

$$W[j] = \mathcal{A}[\phi_{\rm cl}] + \phi_{\rm cl} j + \hbar\Delta_1[\phi_{\rm cl}] \tag{14.71}$$

and prerequisited the perturbation expansion

$$\Delta_1[\phi_{\rm cl}] = \frac{i}{2}{\rm Tr}\,\log i\mathcal{D}^{-1} + \hbar W_2[\phi_{\rm cl}]. \tag{14.72}$$

The functional $W[j]$ depends explicitly on j only via the second term, in all others the j dependence is due to $\phi_{\rm cl}[j]$. We may use this fact by expressing j as a function of $\phi_{\rm cl}$ and writing

$$W[\phi_{\rm cl}] = \mathcal{A}[\phi_{\rm cl}] + \phi_{\rm cl}\; j[\phi_{\rm cl}] + \Delta_1. \tag{14.73}$$

If we now insert (14.50) and use (14.58) we find

$$\begin{aligned}\Gamma[\Phi] &= \mathcal{A}[\phi] - \hbar\mathcal{A}_\Phi[\Phi]\phi_1 - \hbar\phi_1 j[\Phi] + \hbar^2\phi_1 j_\Phi[\Phi]\phi_1 + \frac{1}{2}\hbar^2\phi_1 i\mathcal{D}^{-1}[\Phi]\phi_1 \\ &\qquad +\hbar\Delta_1[\Phi] - \hbar^2\Delta_{1\Phi}[\Phi]\phi_1 + \mathcal{O}(\hbar^3) \qquad (14.74) \\ &= \mathcal{A}[\Phi] + \hbar\Delta_1[\Phi] + \hbar^2\left\{\frac{1}{2}\phi_1 i\mathcal{D}^{-1}[\phi]\phi_1 + \phi_1 j_\Phi[\Phi]\phi_1 - \Delta_{1\Phi}\phi_1\right\}\end{aligned}$$

Let us find the correction Φ_1 to the vacuum expectation value of ϕ. Considering $W[j]$ in (14.60) again as functional in j we see that

$$\Phi = \delta W[j]/\delta j = \phi_{\rm cl} + \hbar\Delta_{1\phi_{\rm cl}}[\phi_{\rm cl}]\delta\phi_{\rm cl}/\delta_j \tag{14.75}$$

such that

$$\phi_1 = \Delta_{1_{\phi_{\rm cl}}}[\phi_{\rm cl}]\delta\phi_{\rm cl}/\delta_j. \tag{14.76}$$

But the derivative $\delta\phi_{\rm cl}/\delta_j$ is known from

$$\delta_j/\delta\phi_{\rm cl} = -\mathcal{A}_{\phi\phi}[\phi_{\rm cl}] = -i\mathcal{D}^{-1}[\phi_{\rm cl}] \tag{14.77}$$

such that

$$\phi_1 = \Delta_{1\phi_{\rm cl}}[\phi_{\rm cl}] i\mathcal{D}[\phi_{\rm cl}]. \tag{14.78}$$

Inserting these equations into (14.74), the $\hbar^2$-term becomes

$$-\frac{\hbar^2}{2}\phi_1 i\mathcal{D}^{-1}[\Phi]\phi_1 + \mathcal{O}(\hbar^3). \tag{14.79}$$

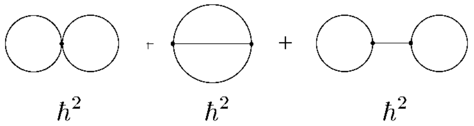
In the derivative Δ_{1_ϕ}, only the trace log term in (14.61) has to be included, to this order in $\hbar$, so that the effective action becomes

$$\begin{aligned}\Gamma[\Phi] &= \mathcal{A}[\Phi]+\hbar\Gamma_1[\Phi]+\hbar^2\Gamma_2[\Phi]\\ &= \mathcal{A}[\Phi]+\frac{i}{2}\mathrm{Tr}\,\log i\mathcal{D}^{-1}[\Phi]+\hbar^2W_2[\Phi]\\ &\quad -\frac{\hbar^2}{2}\frac{i}{2}\mathrm{Tr}\left(\mathcal{D}\frac{\delta}{\delta\Phi}\mathcal{D}^{-1}\right)i\mathcal{D}\frac{i}{2}\mathrm{Tr}\,\mathcal{D}\frac{\delta}{\delta\Phi}\mathcal{D}^{-1}.\end{aligned}\tag{14.80}$$

Let us now calculate W_2 to lowest order in $\hbar$. The remainder I in (14.69) has the expansion

$$I[\Phi;\phi]=\frac{1}{3!}\phi^3\mathcal{A}_{\Phi\Phi\Phi}[\Phi]+\frac{1}{4!}\phi^4\mathcal{A}_{\Phi\Phi\Phi\Phi}[\Phi],$$

where we have replaced $\phi_{\rm cl}$ by $\Phi+\mathcal{O}(\hbar)$. In order to obtain W_2, we have to calculate all connected vacuum diagrams for the interactions r with a ϕ-particle propagator $\dot{\phi}\dot{\phi}=\hbar\mathcal{D}[\Phi]$. Since every contraction brings in a factor $\hbar$, we can truncate the expansion (14.81) after Φ^4. Thus the only contribution to $W_2[\Phi]$ are the connected vacuum diagrams



(14.81)

where a line stands now for $\mathcal{D}[\Phi]$, a four-vertex for

$$\mathcal{A}_{\Phi\Phi\Phi\Phi}[\Phi]=i\mathcal{D}^{-1}[\Phi]_{\Phi\Phi},\tag{14.82}$$

and a three-vertex for

$$\mathcal{A}_{\Phi\Phi\Phi}[\Phi]=i\mathcal{D}^{-1}[\Phi]_{\Phi}.\tag{14.83}$$

Only the first two graphs are one-particle irreducible. It is now a pleasant feature that the third graph cancels with the last term in (14.80). In order to see this we write the diagram more explicitly as

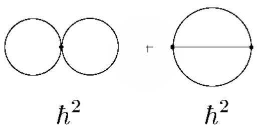
$$-\frac{\hbar^2}{8}\mathcal{D}_{\Phi_1\Phi_2}\mathcal{A}_{\Phi_1\Phi_2\Phi_3}\mathcal{D}_{\Phi_3\Phi_{3'}}\mathcal{A}_{\Phi_{3'}\Phi_{1'}\Phi_{2'}}\mathcal{D}_{\Phi_{1'}\Phi_{2'}}\tag{14.84}$$

which is now part of iW_2. Thus, only the one-particle irreducible vacuum graphs as make up the $\hbar^2$-correction to $\Gamma[\Phi]$:

$$i\hbar^2\Gamma_2[\Phi] = i\hbar^2\frac{3}{4!}\mathcal{D}_{12}\mathcal{A}_{\Phi_1\Phi_2\Phi_3\Phi_4}\mathcal{D}_{34}+i\hbar^2\frac{1}{4!^2}\mathcal{A}_{\Phi_1\Phi_2\Phi_3}\mathcal{D}_{\Phi_1\Phi_{1'}}\mathcal{D}_{\Phi_2\Phi_{2'}}\mathcal{D}_{\Phi_3\Phi_{3'}}\mathcal{A}_{\Phi_1\Phi_2\Phi_3}\tag{14.85}$$

whose graphical representation is

$$i\hbar^2\Gamma_2[\Phi] =$$



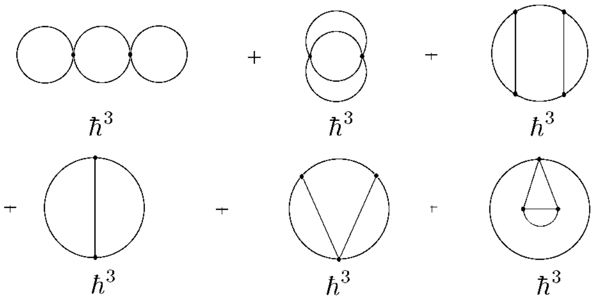
(14.86)

This topological property of the diagram is true for arbitrary orders in $\hbar$. To calculate Γ, we define fundamental vertices of nth order

$$\mathcal{A}_{\Phi_1\ldots\Phi_n}[\Phi],$$

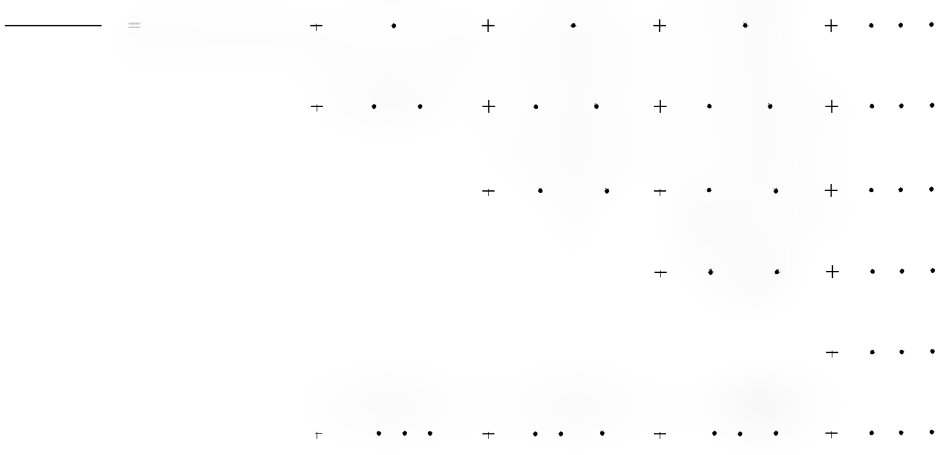
and sum up all connected one particle irreducible vacuum graphs [4]

$$\sum_{n\geq 2} i\hbar^n\Gamma_n[\Phi] =$$



(14.87)

Note the content of the lines $\mathcal{D}$ in terms of fundamental Feynman diagrams. The lines in these diagrams contain infinite sums of diagrams in the original perturbation expansion. If propagators of the original ϕ-theory are indicated by a dashed line, an expansion of $\mathcal{D}$ in powers of Φ reveals that every line corresponds to a sum



(14.88)

line emits $1, 2, 3\ldots$ lines via vertices ϕ^n in arbitrary combinations.

The expansion to order $\hbar^n$ is an expansion according to the number of loops.

The general structure of the series (14.87) becomes rapidly involved functional formalism. It is treated in the next section.

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[4] Note that each line carries a factor $\hbar$ from the propagator, the n-vertex contributes a factor $\hbar^{1-n}$.

14.5 Effective Action to all Orders in $\hbar$

In order to find the general loop expansion, let us expand Φ not around the classical colution $\phi_{\rm cl}$ but around some other functional $\phi_0 = \phi_0[j]$ whose properties will be specified later. Then the generating functional is

$$Z[j] = e^{\frac{i}{\hbar}W[j]} = \mathcal{N}e^{\{\frac{i}{\hbar}\mathcal{A}[\phi_0]+\phi_0 j+\hbar\Gamma_1[\phi_0[j]]\}} \tag{14.89}$$

where

$$e^{\frac{i}{\hbar}\Gamma_1[\phi_0]} \equiv \int \mathcal{D}\phi' e^{\frac{i}{\hbar}\{\mathcal{A}[\phi_0+\phi']-\mathcal{A}[\phi_0]+j[\phi_0]\phi'\}}. \tag{14.90}$$

On the right-hand side we have inverted the relation $\phi_0[j]$ and expressed j as a functional of Φ_0. The field Φ may be calculated as

$$\Phi = \frac{\delta W[j]}{\delta j} = \phi_0 + \left\{\frac{\delta\mathcal{A}[\phi_0]}{\delta\phi_0} + j + \hbar\frac{\delta\Gamma_1[\phi_0]}{\delta\phi_0}\right\}\frac{\delta\phi_0}{\delta j}. \tag{14.91}$$

Since ϕ_0 is not equal to $\phi_{\rm cl}$, the first two terms in the bracket do not cancel. Instead, we shall determine ϕ_0 by the requirement that the whole bracket vanishes for $j = j[\phi_0]$

$$\frac{\delta\mathcal{A}[\phi_0]}{\delta\phi_0} + j[\phi_0] + \hbar\frac{\delta\Gamma_1[\phi_0]}{\delta\phi_0} = 0. \tag{14.92}$$

This requirement makes ϕ_0 directly equal to Φ and

$$\Gamma[\Phi] = \mathcal{A}[\Phi] + \hbar\Gamma_1[\Phi]. \tag{14.93}$$

Since $\Gamma_1[\phi_0]$ depends on ϕ_i also via $j[\phi_0]$, equation (14.92) looks impossible to solve. In fact, reinserting (14.92) into (14.90) we can find a pure equation for ϕ_0:

$$e^{i\Gamma_1[\phi_0]} = \int \mathcal{D}\phi' e^{\frac{i}{\hbar}\left\{\mathcal{A}[\phi_0+\phi']-\mathcal{A}[\phi_0]-\phi'\mathcal{A}_{\phi_0}[\phi_0]-\hbar'\phi\Gamma_{1\phi_0}[\phi_0]\phi'\right\}} \tag{14.94}$$

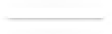
which is a functional integral-different equation. Still it is possible to extract from (14.94) the desired information. Let us consider an auxiliary generating functional

$$e^{iW_{\rm aux}[\phi_0,K]} \equiv \int \mathcal{D}\phi' e^{\frac{i}{\hbar}\left\{\mathcal{A}_{\rm aux}[\phi_0,\phi']+\int d^4x K\phi\right\}} \tag{14.95}$$

with an action

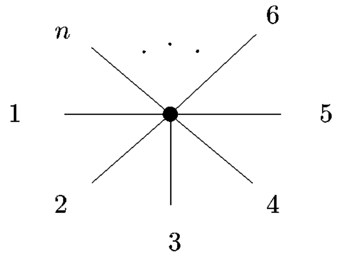
$$\mathcal{A}_{\rm aux}[\phi_0,\phi'] = \mathcal{A}[\phi_0+\phi'] - \mathcal{A}[\phi_0] - \phi'\mathcal{A}\phi_0[\phi_0]. \tag{14.96}$$

It defines, for an arbitrary *fixed* function ϕ_0, an auxiliary field theory with an external source K. If expanded $W_{\rm aux}[K]$ in powers of K, it collects all connected diagrams for the action (14.96). They are built up from propagators



$$= \mathcal{D}[\phi_0] \tag{14.97}$$

and vertices



$$= \frac{\delta^n \mathcal{A}[\phi_0]}{\delta\phi_0 \delta\phi_n \dots \delta\phi_0}. \tag{14.98}$$

Thus, if we succeed in enforcing $\phi_0 = \Phi$, we are dealing exactly with the field theory whose one-particle irreducible vacuum graphs are supposed to make up the corrections $\Gamma_1[\Phi]$. How can we show this? By comparing (14.94) with (14.90) we see that for the special choice of the current

$$K \equiv K_0 - \hbar \Gamma_{1\phi_0}[\phi_0] \tag{14.99}$$

the auxiliary functional $W_{\rm aux}[\phi_0, K_0]$ becomes identical to the generating functional we are trying to calculate. The auxiliary functional also has an auxiliary Legendre transformed field

$$\Phi_{\rm aux} = \frac{\delta W_{\rm aux}[\phi_0, K]}{\delta K}. \tag{14.100}$$

Thus, if we succeed in enforcing $\phi = \Phi$, we are dealing exactly with the field theory whose one-particle irreducible vacuum graphs are supposed to make up the corrections $\Gamma_1[\Phi]$. Indeed, by comparing (14.94) with (14.90) we see that for the special choice of the current

$$K \equiv K_0 - \hbar \Gamma_{1\phi_0}[\phi_0], \tag{14.101}$$

the auxiliary functional $W_{\rm aux}[\phi_0, K_0]$ becomes identical to the generating functional we are trying to calculate.

With the help of

$$\Phi_{\rm aux} = \frac{\delta W_{\rm aux}[\phi_0, K]}{\delta K} = \Phi_{\rm aux}[\phi_0, K] \tag{14.102}$$

we now define an auxiliary effective action

$$\Gamma_{\rm aux}\,[\Phi_{\rm aux}] \equiv W_{\rm aux}[\phi_0, K] - \int d^4x K \Phi_{\rm aux}, \tag{14.103}$$

where $\Gamma_{\rm aux}\,[\Phi_{\rm aux}]$ is also a functional of ϕ_0. There is one important property of $\Gamma_{\rm aux}\,[\Phi_{\rm aux}]$. If it is evaluated at $\Phi_{\rm aux} = 0$, it collects all one-particle irreducible vacuum graphs of $\mathcal{A}_{\rm aux}$ [see (11.45), (11.46)]. But these are exactly the graphs we want. Hence the proof can be completed by showing that the condition $K = K_0 = -\Gamma_{1\phi_0}[\phi_0]$ leads to

$$\Phi_{\rm aux} = 0. \tag{14.104}$$

But this is trivial to see: The condition $K = K_0$ was just made up to enforce $\Phi = \phi_0$. The fluctuating fields ϕ' are the difference between ϕ and ϕ_0:

$$\phi' = \phi - \phi_0 = \phi - \Phi. \tag{14.105}$$

Now $\Phi \equiv \langle\phi\rangle$ implies $\langle\phi'\rangle = 0$. But in the auxiliary theory,

$$\Phi_{\rm aux} \equiv \langle\phi'\rangle \tag{14.106}$$

So that $\Phi_{\rm aux} = 0$, and $W_{\rm aux}[\phi_0, K]$ collects the one-particle irreducible vacuum graphs with propagators and vertices (14.101), (14.102). This completes the proof.

15

Spontaneous Symmetry Breakdown

In the perturbation expansion developed in Chapter 8 the classical ground state carries no field. The associated vacuum state is called normal since it is invariant under all symmetry transformations of the action. There are many physical systems where this is not true. As an example, we shall discuss here the ϕ^4-theory with N components $\phi_1, \dots, \phi_N$ coupled in an O(N)-symmetric way.

15.1 Scalar O(N)-Symmetric ϕ^4-Theory

The Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial\phi_a)^2 - \frac{m^2}{2}\phi_a^2 - \frac{g}{4}\left(\phi_a^2\right)^2. \tag{15.1}$$

This is invariant under all N-dimensional rotations of its components

$$\phi_a \to R_{ab}\phi_b, \tag{15.2}$$

which conserve the length of the field vector $\boldsymbol{\phi} \equiv (\phi_a)$,

$$|\boldsymbol{\phi}| = \sqrt{\phi_a^2}. \tag{15.3}$$

The perturbation expansion of the ϕ^4-theory in Chapters 8 and 9, was based on a Taylor expansion of the total generating functional

$$Z[j] = e^{-i(g/4)\int_{-\infty}^{\infty} dt[-i\delta/\delta j(x)]^4} Z_0[j] \tag{15.4}$$

in powers of the interaction g, where $Z_0[j]$ is the generating functional of the free-field theory with a Lagrangian

$$\mathcal{L}_0 = \frac{1}{2}(\partial\phi_a)^2 - \frac{m^2}{2}\phi_a^2. \tag{15.5}$$

This expansion makes sense only for a positive square mass m^2. Assuming a positive coupling constant g, the classical field potential

$$v(\phi_a) = \frac{m^2}{2}\phi_a^2 + \frac{g}{4}\left(\phi_a^2\right)^2 \tag{15.6}$$

has a minimum at the O(N)-symmetric field configuration $\phi_a = \phi_a^0 = 0$. Only in this case can the perturbation expansion of the second-quantized field theory, proceed around the free-field theory described by $\mathcal{L}_0$,

A non-trivial and physically very important situation is, however, described by the case $m^2 < 0$ (at $g > 0$). Then the classical field configuration minimizing $\mathcal{L}$ is given by a nonzero field

$$\phi_a^0 \neq 0. \tag{15.7}$$

This happens in various many-body systems, where field theories of the type (15.6) are used to describe orientational properties of materials, for instance the direction of magnetization. In that case $n = 3$, and the vector (ϕ_1, ϕ_2, ϕ_3) is identified with the local size and orientation of the local magnetization. The generating functional

$$Z[j] = \int \mathcal{D}\phi e^{i\int dx[\mathcal{L}(\phi,\partial\phi)+j_a\phi_a]} \tag{15.8}$$

can serve to understand the fluctuation phenomena in such systems. When comparing theory and experiment it turns out that there is usually a certain temperature T_c, above which the system can be described via the perturbation expansion given in the last chapter. As the temperature is lowered toward T_c, flucuations increase drastically. This can be accounted for in the field theory by letting the mass parameter be temperature dependent such that m^2 vanishes for some temperature $T = T_c^{\rm MF}$, say

$$m^2 = \mu^2 \left(\frac{T}{T_c^{\rm MF}} - 1 \right) \equiv \mu^2 \tau \tag{15.9}$$

where μ is some mass scale. In the bare mass, the temperature carries a superscript MF to indicate that it is the places where the *bare mass* changes sign, and the mean-field approximation has its phase transition. The fluctuations will shift this temperature downwards, making the true critical temperature T_c smaller than T_c. In the low-temperature phase, the directon of the spin vectors ϕ_a is no more random but the system settles at a specific non-zero expectation value of the field which we denoted before as

$$\Phi_a \equiv \langle 0|\phi_a|0\rangle. \tag{15.10}$$

For example, magnetic systems acquire a certain spontaneous magnetization. Eq. (15.10) introduces a new qualitative feature into the theory. The ground state no longer has the symmetry which was contained in the action. A rotation O(N) changes the direction of the ground state just as a magnet can be rotated in space. One speaks of a *spontaneous breakdown* of the original symmetry of the action.

The perturbative calculation order by order cannot account for this feature since, as we have seen, the evenness of the ϕ^4 interaction prevents the existence of any odd-point function. The effect must therefore be due to a non-perturbative mechanism.

It is gratifying to note that this does not prevent us from giving a theoretical explanation of this phenomenon using perturbation-theoretic techniques. In fact, the effective action calculated in the proceeding chapters from such techniques is the ideal tool for this purpose. First of all we notice that whatever symmetry is carried by the action $\mathcal{A}[\phi_a]$, this will also wind up in the effective action $\Gamma[\Phi_a]$. For if $\mathcal{A}[\phi_a]$ does not change under the transformation (15.2), then $W[j_a]$ is invariant under $j_a \to R_{ab}j_b$. Thus $\Phi_a \equiv \delta W/\delta j_a$ transforms according to the same law as ϕ_a and $\Gamma[\Phi_a] = W[j_a] - j_a\Phi_a$ must also be invariant.

This statement is obvious at the lowest-order approximation to the effective action which is equal to the classical action $\mathcal{A}[\phi_a]$ taken at Φ_a:

$$\Gamma[\Phi_a] \approx \mathcal{A}[\Phi_a]. \tag{15.11}$$

At a constant field expectation Φ_a, this determines the effective potential

$$\Gamma[\Phi_a] = -Vv(\Phi_a), \tag{15.12}$$

where $V = d^Dx$ is the spacetime volume. For the Lagange density (15.6), the effective potential is

$$v(\Phi_a) = \frac{1}{2}m^2\Phi_a^2 + \frac{g}{4}\left(\Phi_a^2\right)^2. \tag{15.13}$$

Already at this lowest approximation, the effective action is capable of describing a spontaneous symmetry breakdown. As long as $m^2 > 0$, this has an $O(N)$-symmetric minimum at a single field point, the origin $\Phi_a = 0$. But if m^2 is lowered and becomes smaller than zero, the origin becomes unstable and the potential looks as shown in (15.1). The $O(N)$-symmetry of the potential gives rise to an infinitely degenerate

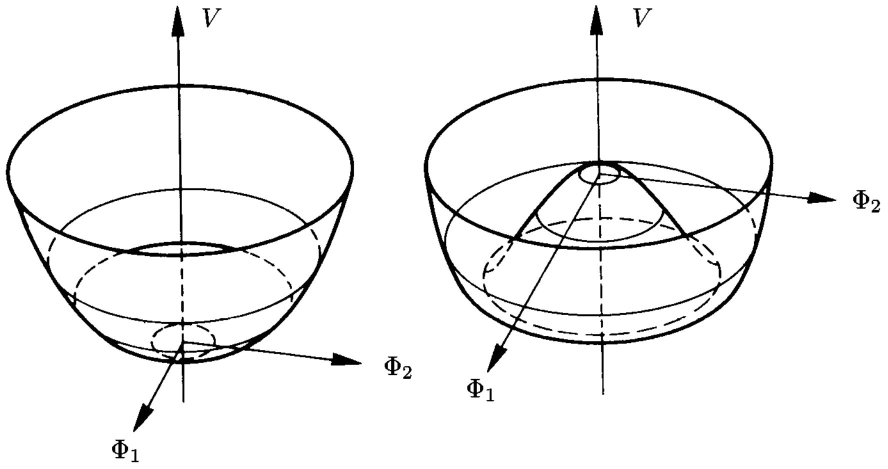


FIGURE 15.1 Effective potential of the ϕ^4-theory for $N = 2$ in mean-field approxmation. for $m^2 > 0$ and $m^2 < 0$, corresponding to temperatures above and below the critical temperature respectively.

minimum characterized by a fixed length of the field vector Φ_a:

$$|\mathbf{\Phi}^0| \equiv \sqrt{\Phi_a^{0\,2}} = \sqrt{\frac{-m^2}{g}}. \tag{15.14}$$

The direction of this minimum can be changed arbitrarily by an O(N)-rotation. without chaning the energy.

The system is unstable at the origin. Small fluctuations which are neglected within the present classical approximation will drive the field down to a new minimum at Φ_0. The non-perturbative aspect of the solution manifests itself in the power $1/\sqrt{g}$ appearing even at the level of no fluctuations.

Notice how the symmetry is spontaneously broken: The system has now many directions to choose from since there is the whole surface of an O(N) sphere ("O(N) shell") of equal $|\mathbf{\Phi}^0|$ which has been pictured in (15.1) as a circle. One says that for $m^2 < 0$ the vacuum is infinitely degenerate. As soon as Φ_a has made its choice, the ground state has lost its symmetry.

From (15.14) we can calculate how the strength of the magnetization varies with temperature using (15.9):

$$|\mathbf{\Phi}^0| = \frac{\mu}{\sqrt{g}}\sqrt{-\tau} = \frac{\mu}{\sqrt{g}}\sqrt{1 - \frac{T}{T_c^{\rm MF}}}.$$

Experimentally, one finds a power law slightly different from this

$$|\mathbf{\Phi}^0| \propto (-\tau)^\beta. \tag{15.15}$$

The power β is defined as the *critical exponent* or *critical index* of this behaviour. For most materials β lies in the vicinity of 1/2 but is not equal to it. Since (15.11) is the mean field approximation to the effective action, the number $\beta = 1/2$ is referred to as the *mean field approximation* to β. It is plotted in Fig. 15.2.

The deviation of β from 1/2 must be due to fluctuations. As a matter of fact, in Section 21.8 we shall derive that for $N = 1$, the one-loop corrections can be described approximately for small m^2 as a change of m^2 to $\mu^2\left(\frac{m^2}{\mu^2}\right)^\gamma$ and of $g\Phi^4$ to $g\left(\frac{m^2}{\mu^2}\right)^{\gamma-2\beta}\Phi^4$ [it is an expansion of a general scaling relation to be derived in Eq. (21.177)]. Anticipating this result in v, we write

$$v(\Phi) = \mu^2\left(\frac{m^2}{\mu^2}\right)^\gamma \Phi^2 + \frac{g}{4}\left(\frac{m^2}{\mu^2}\right)^{\gamma-2\beta}\left(\Phi^2\right)^2 + \mathcal{O}\left(\Phi^6\right). \tag{15.16}$$

But this expression is valid for positive m^2. What can we say about $m^2 < 0$? Looking at the original one-loop formula we see that the whole effective action can be continued analytically to negative m^2 as long Φ^2 is kept nonzero, so that

$$m^2 + \frac{g}{2}\Phi^{0\,2} > 0. \tag{15.17}$$

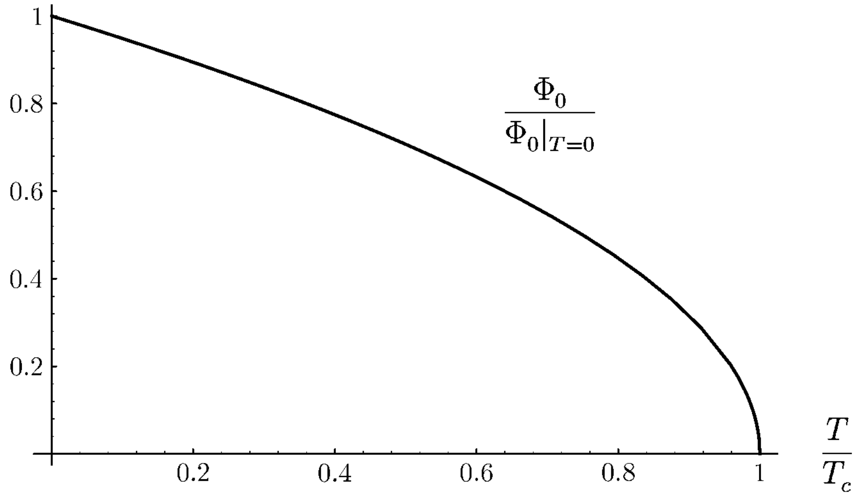


FIGURE 15.2 Magnetization Φ_0 in mean-field approximation as a function of the temperature ratio $T/T_c^{\rm MF}$ in mean-field approximation.

But this is too close to the new minimum which with the normalization of the coupling used there ($g_{\rm old} = 3! g_{\rm new}$) was at

$$\Phi^{02} = -\frac{m^2}{g} 3! \tag{15.18}$$

such that $m^2 + g\Phi^2/2 = -2m^2 > 0$. Moreover, the full loop expansion formula to all orders can be calculated for Φ close to this minimum since all propagators $\mathcal{D} = i/\left(-\partial^2 - m^2 - g\Phi^2/2\right)$ correspond to particles of proper positive mass term. Also: The renormalization program needs no modification. The same counter terms which made the results finite above $T_c^{\rm MF}$ keep the results finite below $T_c^{\rm MF}$. We only have to forbid Φ to drop.

The only point to watch out is that the Φ never drops below a certain critical value

$$\Phi^2 < \Phi^{c2} = \frac{1}{3}\Phi^{02} = -2\frac{m^2}{g} \tag{15.19}$$

at which place logarithms pick up negative arguments and give rise to imaginary parts. Thus, as long as we avoid the critical value (15.19) we may use (15.16) also for $m^2 < 0$, $T < T_c^{\rm MF}$. Actually, that result was derived only for a single Φ field. But it can easily be shown that the same form remains also for the O(N) field Φ_a except with slightly different numbers for the powers β, γ.

We may now use (15.16) for the same discussion as carried through previously and find now a vacuum expectation below $T_c^{\rm MF}$ of

$$|\mathbf{\Phi}^0| = \left(-\frac{m^2}{g}\right)^\beta = (-\tau)^\beta. \tag{15.20}$$

By comparing this one-loop corrected theoretical result with experiment one does find an improvement in the right direction.

The theory of critical indices has been the subject of many investigations in the past years. Therefore they deserve a more detailed discussion which will be given in a separate chapter. Let us end this section by pointing out that the appearance of an imaginary part for $\Phi^2 < \Phi_c^2$ has a good physical reason: Imaginary parts in an energy are always related to an instability of the system. The origin of the instability for $\Phi^2 < \Phi_c^2$ can easily be found: Let us turn on an external field j which drives Φ into the region of instability. The effective potential becomes

$$v(\Phi) = \frac{m^2}{2}\Phi^2 + \frac{g}{4!}\Phi^4 - j\Phi \tag{15.21}$$

and looks as plotted in (15.1).

The value of Φ at the minimum increases with j. The other minimum at the diametrally opposite place, however, begins to move closer to the axis. We can display the two minima as a function of j by plotting the derivative of $v(\Phi)$, (see (15.3)

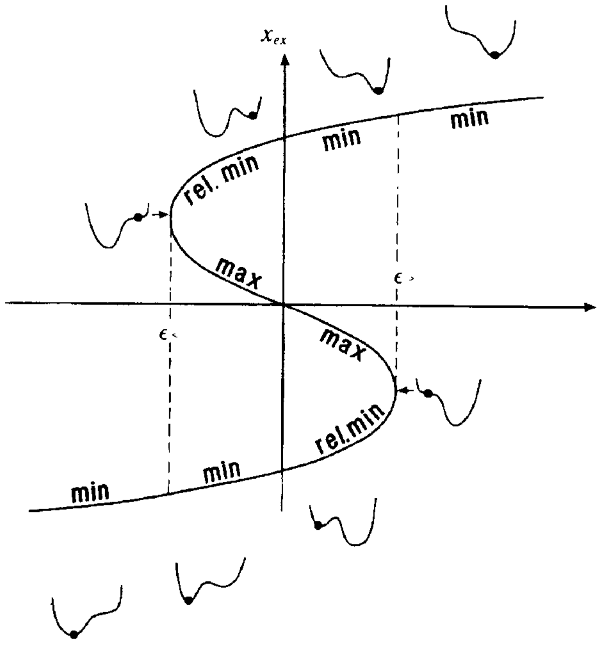


FIGURE 15.3 Magnetization Φ_0 as a function of external source j in mean-field approximation.

$$j = m^2\Phi + \frac{g}{3!}\Phi^3. \tag{15.22}$$

For very large j or $-j$, there is only a single minimum on the right or left-hand side, respectivly. In a region $|j| \leq j_c$ there are three solutions, two minima and a maximum. The value j_c is determined from the maximum of the curve (15.22)

$$j_c = -\sqrt{\frac{2m^2}{g}\frac{2}{3}m^2} \tag{15.23}$$

which lies at

$$\Phi^{c2} = -2m^2/g. \tag{15.24}$$

There the minimum fuses with the maximum and disappears. But this is precisely the place at which the effective potential develops an imaginary part. Thus the instability indicated by the appearance of an imaginary part in the effective potential is simply a signal for the fact that the local minimum at the elevated place can no longer be a solution of the field equation. The point becomes locally unstable. Notice that the same instability point appears to all orders in the loop expansion, i. e. to all orders in the fluctuation expansion.

From our knowledge of simple quantum mechanical systems we may conclude that this result cannot contain the whole truth about the instability. While the system certainly can be in the higher minimum, it alsways has a possibility of escaping through the potential barrier via tunneling. Thus there must be an imaginary part in the true effective potential as soon as $|\Phi| < |\Phi^0|$. Obviously, the loop expansion cannot account for this. Even the hope that a full summation of all terms might produce a corresponding singularity at $\Phi = \Phi^0$ is futile. From quantum mechanics it is known that tunneling amplitudes behave as $e^{-a/g\hbar}$. But such an expression can never be recovered from a loop expansion in a power series in g. (The power series expansion of $e^{-a/g\hbar}$ would be $1 + 0 + 0 + \ldots$). Methods to describe physical effects of this type will be developed in a later chapter.

15.2 Nambu-Goldstone Particles

15.2.1 The Mechanism

There is an important physical consequence of spontaneous symmetry breakdown. The system has an infinite choice between different directions of ϕ. Consider a field configuration which is not constant in space but changes smoothly from space-time point to space-time point along the degenerate O(N) shell. Obviously, the energy of such a configuration can be made arbitrarily small. But this means that there is a large region in field space over which fluctuations hardly change the action. Thus the suppression of fluctuation cannot be very effective and the angular fluctuations of the field are large. Let us see this explicitly for the case $N = 2$ for which ϕ may be written as a single complex field $\phi = \phi_1 + i\phi_2$. Going to a radial decomposition

$$\phi = \rho e^{i\gamma} \tag{15.25}$$

we may write the action as

$$\mathcal{A}[\phi] = \frac{1}{2}(\partial\rho)^2 - \frac{m^2}{2}\rho^2 + \frac{1}{2}\rho^2(\partial\gamma)^2 - \frac{g}{4}\rho^4. \tag{15.26}$$

For $m^2 < 0$, consider variations of ρ around $\rho_0 = \sqrt{-m^2/g}$. If $\gamma(\mathbf{x})$ is kept constant we may expand $\rho = \rho_0 + \delta\rho$ and write

$$\delta^2\mathcal{A}[\phi] = \frac{1}{2}(\partial\delta\rho)^2 + \frac{2m^2}{2}(\delta\rho)^2. \tag{15.27}$$

Notice that the size fluctuations $\delta\rho$ take place with a mass twice the opposite of the $T > T_c^{\rm MF}$ case.

An O(2)-symmetric field theory with ϕ^4-interaction can be used to describe the phase transition from normal to superfluid in liquid helium near 2.7 degrees Kelvin.

The O(2) degeneracy of the ground state manifests itself in the independence of the action on γ as long as it is constant. If γ has small space time variations we may write $\gamma = \gamma_0 + \delta\gamma$ and get an additional piece in the action (to quadratic order)

$$\delta^2\mathcal{A}[\phi] = \frac{1}{2}{\rho_0}^2(\partial\delta\gamma)^2. \tag{15.28}$$

Consider now the eigenmodes of quadratic fluctuations. Previously, for $m^2 > 0$, we had two (in general N) particles both (all) of mass m. Now we have one field $\delta\rho$ with propagator

$$G_{\delta\rho\delta\rho} = \frac{i}{-\partial^2 + 2m^2} \tag{15.29}$$

and another field $\delta\gamma$ with propagator

$$G_{\delta\gamma\delta\gamma} = \frac{1}{{\rho_0}^2}\frac{i}{-\partial^2}. \tag{15.30}$$

This is a massless particle called Nambu-Goldstone boson whose presence in the case of spontaneously broken symmetry was first discovered by Nambu, followed by a more rigorous treatment by Goldstone.

Remember that the physical origin is the arbitrarily small change of action for smooth continuous variations of the ground state directions.

At long distances, the only experimantal correlations come from the massless modes. There exist many physical phenomena which are dominated by these. They can be studied approximately by ignoring completely the variations of the size of the field ρ, freezing it at the equilibrium value ρ_0. This is called the *hydrodynamic limit* of the field theory. It describes only the Nambu-Goldstone boson. In the O(N)-symmetric theory, the freezing of the size of the field leaves the directional vector $n_a = \phi_a/|\phi|$ free to fluctuate. Then the field theory model goes over into the classical Heisenberg model.

This limit will be discussed further in Section 19.

15.2.2 General Considerations

The necessity of a Nambu-Goldstone particle as a consequence of spontaneous symmetry breakdown can easily be proved for any continous symmetry and to all orders in perturbation theory by using the full effective action. Let us look only at the case of O(N) symmetry. The infinitesimal symmetry transformation on the currents are

$$j_a \to j_a - i\epsilon_{cd}\left(L_{cd}\right)_{ab} j_b \tag{15.31}$$

where L_{cd} are the $N(N-1)/2$ generators of O(N) rotations. Under this, the generating functional is invariant

$$\delta W[j] = \int dx \frac{\delta W[j]}{\delta j_a(x)} i\left(L_{cd}\right)_{ab} j_b \epsilon_{cd} = 0. \tag{15.32}$$

Let us insert the Legendre tranformation laws for Φ and j. Then (15.32) amounts to

$$0 = \int dx \Phi_a(x) i\left(L_{cd}\right)_{ab} \frac{\delta\Gamma[\Phi]}{\delta\Phi_b(x)}\epsilon_{cd} \tag{15.33}$$

which expresses the infinitesimal invariance of the effective action under

$$\Phi_a \to \Phi_a - i\epsilon_{cd}\left(L_{cd}\right)_{ab}\Phi_b.$$

The invariance law (15.33) is often called the *Ward-Takakashi identity* for the functional $\Gamma[\Phi]$. It can be used to find an infinite set of identities with this name for all the vertex functions by forming higher functional derivatives and setting $\Phi = \Phi^0$ at the end. For example the first derivative of (15.33) gives (dropping the infinitesimal parameter ϵ_{cd})

$$0 = \left(L_{cd}\right)_{ab}\frac{\delta\Gamma[\Phi]}{\delta\Phi_b(x)} + \int dx' \Phi_{a'}(x')\left(L_{cd}\right)_{a'b}\frac{\delta^2\Gamma[\Phi]}{\delta\Phi_b(x')\delta\Phi_a(x)}. \tag{15.34}$$

Setting $\Phi = \Phi^0$ where $j_a = \delta\Gamma[\Phi]/\delta\Phi_b(x) = 0$ gives

$$\int dx' \Phi^0_{a'}(x)\left(L_{cd}\right)_{a'b}\frac{\delta^2\Gamma[\Phi^0]}{\delta\Phi^0_b(x')\delta\Phi^0_a(x)}$$

At $\Phi = \Phi^0$, the second derivative of $\Gamma[\Phi^0]$ is simply the vertex function $\Gamma^{(2)}$ at zero momentum which in turn, by (??)), equals the inverse of the connected two-point function in momentum space $G(p)$. Hence we obtain

$$\Phi^0_{a'}\left(L_{cd}\right)_{a'b}[G_c^{-1}]_{ba}(q=0) = 0. \tag{15.35}$$

This statement implies that certain fully interacting propagators have to contain a singularity at $q = 0$. In most cases this caused by a pole in the variable q^2.

Then (15.35) implies the existence of a massless particle in the Hilbert space, the Nambu-Goldstone boson. We shall see later what exceptions there can be.

We have argued before that the directions of massless fluctuations must be associated with the valley of degeneracy in the effective potential. Eq. (15.35) is a mathematical expression of this observation. As an example consider the case $N=2$. Then $(L_{cd}\epsilon_{cd})_{ab}$ is simply the 2×2-matrix

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \epsilon_{12}$$

Let the vacuum expectation of the two-component field $\phi_a(x)$ be

$$\Phi^0 = \left(\Phi^0, 0\right).$$

Then (15.35) states that

$$[G_c^{-1}]_{22}\,(q=0) = 0, \qquad (15.36)$$

calling for a massless mode along the second field direction. Translating this into the complex field language studied previously, we rewrite $\Phi_a = (\rho\cos\gamma,\ \rho\sin\gamma)$ as

$$\Phi = \rho e^{i\gamma}.$$

For ρ close to ρ_0 and small γ, this is precisely the massless mode in the azimuthal variable. For $N=3$, the rotation may be written as

$$(L_{cd}\epsilon_{cd})_{ab} = -\epsilon_{dab}\alpha_d,$$

where α is a small angle of rotation and $\epsilon_{123}=1$. Then (15.35) becomes

$$\epsilon_{abd}\Phi_a^0[G_c^{-1}]_{bc}(q=0) = 0. \qquad (15.37)$$

For Φ_a^0 pointing in 3-direction, the modes $[G_c]_{11}^{(2)}$ and $[G_c]_{22}^{(2)}$ are massless.

Note that only statements on diagonal elements are non-trivial since $[G_c^{(2)}]_{ij}$ vanishes unless $i=j$, as is obvious at the one-loop level and can be shown to hold for any invariant power $\left(\Phi_a^2\right)^n$ appearing in the effective action.

The Goldstone mode has an exception which has turned out to provide the basis of present theories of weak interactions. It therefore deserves being discussed in detail in the next section.

15.2.3 Experimental Consequences

The Nambu-Goldstone phenomenon has important observational consequences. The most simple experiment which can be done on a system is to study the change of the energy as a function of an external field j. The object

$$\frac{\delta W[j]}{\delta j} = \langle 0|\phi(x)|0\rangle_{j=\text{const}} = \Phi \qquad (15.38)$$

is observable directly as an order parameter of the system (say magnetization). The change of this order parameter with respect to changes in j

$$\frac{\delta\Phi(x)}{\delta j(y)} = \frac{\delta^2 W[j]}{\delta j(x)\delta j(y)} = \langle 0|T\phi(x)\phi(y)|0\rangle = \chi(x,y)$$

is measured as a susceptibility. Its Fourier transform

$$(2\pi)^4\delta^{(4)}(q+q')\chi(q) = \int d^4x \int d^4x' e^{i(qx+q'x')}\chi(x,x') \tag{15.39}$$

at $q_0 = 0$ is called the static susceptibility. Using our identities of Ch. 6, we may write equivalently

$$(2\pi)^4\delta^{(4)}(q-q')\chi^{-1}(q) = -\frac{\delta^2\Gamma[\Phi]}{\delta\Phi_a(q)\delta\Phi_b(q')}, \tag{15.40}$$

or

$$\chi^{-1}(0) = \frac{\partial^2 v}{\partial\Phi_a\partial\Phi_b}. \tag{15.41}$$

Let us calculate these quantities at the mean-field level. For $\tau > 0$ we find

$$\begin{aligned} \chi_{ab}^{-1}(q) &= \left(m^2 + \mathbf{q}^2 - q_0^2\right)\delta_{ab} = \left(\mu^2\tau + \mathbf{q}^2 - q_0^2\right)\delta_{ab} \\ \chi_{ab}^{-1}(0) &= m^2\delta_{ab} = \mu^2\tau\delta_{ab}. \end{aligned} \tag{15.42}$$

Thus χ^{-1} increases linearly with τ and is a favorite quantity for experimental plots. Very close to a critical point, the measurements show deviations from this law due to fluctuations. Near $T = T_c^{\mathrm{MF}}$, one measures a power law parametrized by

$$\chi_{ab}^{-1} = \mu^2\tau^\gamma\delta_{ab}.$$

The value of γ is called the the *critical index* of susceptibility above T_c^{MF}. The derivation of this power behavior will be given in Subsec. 21.9.1 [see Eq. 21.155)].

As the temperature passes below T_c^{MF}, the spontaneous breakdown of O(N) symmetry leads to a drastic change: The susceptibility $\chi_{ab}(q)$ looses its isotropy in filed space. The component longitudinally to the direction Φ_a^0 behaves like

$$\begin{aligned} \chi_{11}^{-1}(q) &= -2m^2 + q^2 - q_0^2 = -2\mu^2\tau + q^2 - q_0^2 \quad \tau < 0 \\ \chi_{11}^{-1}(0) &= -2m^2 = -2\mu^2\tau \quad \tau < 0. \end{aligned} \tag{15.43}$$

Then N transverse components of χ_{ab}^{-1}, on the other hand, vanish at $q = 0$ (see (15.35)) since

$$\chi_\perp^{-1}(q) = G^{-1}(q) = q - q_0^2. \tag{15.44}$$

Thus $\chi_\perp$ diverges for $q \to 0$ and this leads to a dramatic experimental effect: If the external source describes incoming waves with weak space-time dependence, the system scatters these very strongly. For example, if j corresponds to an electromagnetic field in the optical range (as is the case in nematic liquid crystals) the system becomes completely opaque (it looks milky). When cooling through $T_c^{\rm MF}$ this phenomenon is called *critical opalescence.*

Notice that a spontaneously broken *continuous* symmetry is necessary for the opalescence below $T_c^{\rm MF}$. In the case of a single real ϕ field (Ising like system) there are no Goldstone modes and there is no $\chi_\perp^{-1}$ which stays identically zero for $T < T_c^{\rm MF}$, $q = 0$. There, one sees critical opalescence just in the immediate vicinity of $T_c^{\rm MF}$ and the system becomes again clear below $T_c^{\rm MF}$.

15.3 Domain Walls in O(1)-Symmetric Theory

The field equations following from the Lagrangian (15.6) are

$$\left[\partial^2 + m^2 + g\phi_b^2(x)\right]\phi_a(x) = 0. \tag{15.45}$$

For $m^2 < 0$, where the potential looks like the bottom of a champaign bottle in Fig. 15.1, these equations possess nontrivial static solutions solving the spatial part of the differential equation (15.45):

$$\left[-\boldsymbol{\partial}^2 + m^2 + g\phi_b^2(\mathbf{x})\right]\phi_a(\mathbf{x}) = 0. \tag{15.46}$$

The simplest nontrivial solution varies only along one axis, say the x-axis, and only in one field component. It will turn out to be a stable solution only if the ather components are absent altogether. There the Lagrangian (15.6) possesses merely a repfection symmetry $\phi \longrightarrow -\phi$, which in the general context is called O(1)-symmetry.

Thus we shall study the simplified field equation

$$\left[-\frac{d^2}{dx^2} + m^2 + g\phi^2(x)\right]\phi(x) = 0. \tag{15.47}$$

For a single field component, the potential has the form of a double-well pictured in Fig. 15.4. The equation (15.47) has two trivial constant solutions

$$\phi(x) \equiv \pm\phi_0 \equiv \sqrt{\frac{-m^2}{g}} \tag{15.48}$$

which lie at the two minima of the potential

$$V(\phi) = \frac{m^2}{2}V(x) = \frac{m^2}{2}\phi^2 + \frac{g}{4}\phi^4. \tag{15.49}$$

At the minimum, the potential has the value

$$V_c = -\frac{m^4}{g}, \tag{15.50}$$

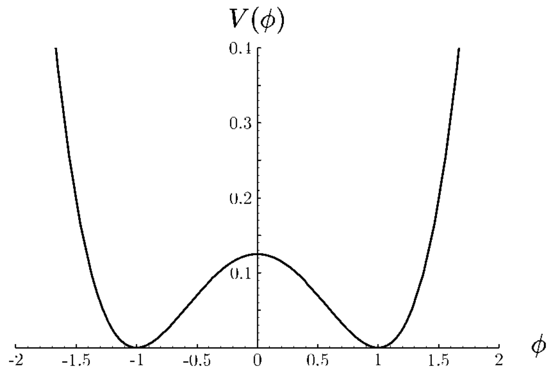


FIGURE 15.4 Plot of the symmetric double-well potential $V(x) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4$. We have added a trivial constant 1/4 to place the minima on the ϕ-axis.

which is called the *condensation energy* of the field system. It will be convenient to subtract this from $V(\phi)$ and write the subtracted potential

$$V(\phi) = \frac{m^2}{8\phi_0^2}(\phi - \phi_0)^2(\phi + \phi_0)^2, \tag{15.51}$$

exhibiting more directly the symmetric minima at $\phi = \pm\phi_0$ (see Fig. 15.4). The coupling strength is

$$g = m^2/2\phi_0^2. \tag{15.52}$$

Near the minima, the potential looks approximately like a harmonic oscillator potential $V_\pm(\phi_0) = m^2(x \mp \phi_0)^2/2$:

$$V(\phi) = \frac{m^2}{2}(\phi \mp \phi_0)^2 \left(1 \pm \frac{\phi \mp \phi_0}{\phi_0} + \ldots\right) \equiv V_\pm(\phi) + \Delta V_\pm(\phi) + \ldots\,. \tag{15.53}$$

The height of the potential barrier at the center is

$$V_{\max} = \frac{(m\phi_0)^2}{8}. \tag{15.54}$$

In the limit $\phi_0 \to \infty$ at a fixed frequency m, the barrier height becomes infinite and the system decomposes into a sum of two independent harmonic-oscillator potentials widely separated from each other.

The nontrivial solution of the field equation connects the two trivial solutions (15.48) across the barrier. As we shall derive immediately, this reads

$$\phi(x) = \phi_{\rm cl}^{\pm}(x) \equiv \pm\phi_0 \tanh[m(x - x_0)/2], \tag{15.55}$$

with an arbitrary parameter x_0 specifying the point on the x-axis where the crossing takes place. The crossing takes place over a distance of the order of $2/m$. For large positive and negative x, the solution approaches $\pm\phi_0$ exponentially (see Fig. 15.5).

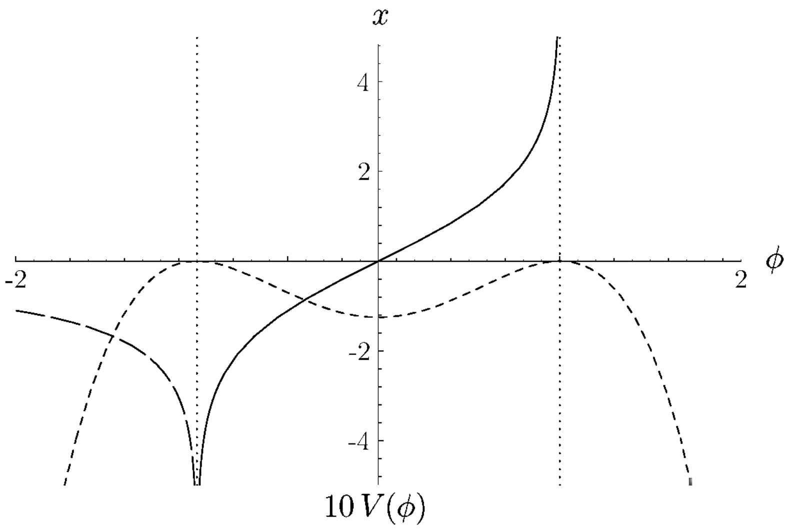


FIGURE 15.5 Classical kink solution (solid curve) in double-well potential (short-dashed curve with units marked on the lower half of the vertical axis). The solution connects the two degenerate maxima in the reversed potential. The long-dashed curve shows a solution which starts out at a maximum and slides down into the adjacent abyss.

The subscript cl on $\phi_{\rm cl}$ emphasized that these solutions solve the classical field equations. In allon to their shape, the solutions $\phi^{\pm}_{\rm cl}(x)$ are called *kink* and *antikink* solutions, respectively.[1]

To derive these solutions, consider the equation of motion (15.47) in the pseudotime time $t = ix$,

$$\ddot{\phi}(t) = -V'(\phi(t)), \tag{15.56}$$

where $V'(\phi) \equiv dV(\phi)/d\phi)$. Since the differential equation is of second order, there is merely a sign change in front of the potential with respect to thr spatial differential equation (15.47). The equation of motion (15.56) corresponds therefore to a usual equation of motion of a point particle as a function of the pseudotime t, whose potential is turned upside down with respect to Fig. 15.4. This is illustrated in Fig. 15.6. The reversed potential allows obviously for a classical solution which starts out at $\phi = -\phi_0$ for $x \rightarrow -\infty$ and arrives at $\phi = \phi_0$ for $x \rightarrow +\infty$. The particle needs an infinite time to leave the initial potential mountain and to climb up to the top of the final one. The movement through the central valley proceeds within the finite time $\approx 2/m$. If the particle does not start its movement exactly at the top but slightly displaced towards the valley, say at $\phi = -a + \epsilon$, it will reach $\phi = a - \epsilon$ after a finite time, then return to $\phi = -a + \epsilon$, and oscillate back and forth forever. In the limit $\epsilon \rightarrow 0$, the period of oscillation goes to infinity and only a single crossing of the valley remains.

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[1] In field-theoretic literature, such solutions are also referred to as instanton or anti-instanton solutions, since the valley is crossed within a short time interval. See the references quoted at the end of the chapter.

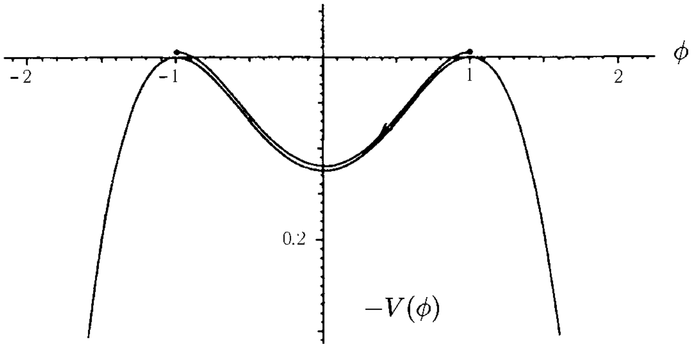

FIGURE 15.6 Reversed double-well potential governing the motion of the position ϕ as a function of the imaginary time x.

To calculate this movement, the differential equation (15.45) is integrated once after multiplying it by $\phi' = dx/dx$ and rewriting it as

$$\frac{1}{2}\frac{d}{dx}x'^2 = \frac{d}{dx}V(\phi(x)). \tag{15.57}$$

The integration gives

$$\frac{x'^2}{2} + [-V(\phi(x))] = \text{const}\,. \tag{15.58}$$

If x is reinterpreted as the physical time, this is the law of *energy conservation* for the motion in the reversed potential $-V(\phi)$. Thus we identify the integration constant in (15.58) as the total energy E in the reversed potential:

$$\text{const} \equiv E. \tag{15.59}$$

Integrating (15.58) further gives

$$x - x_0 = \pm\frac{1}{\sqrt{2}}\int_{\phi(x_0)}^{\phi(x)} \frac{d\phi}{\sqrt{E+V(\phi)}}. \tag{15.60}$$

A look at the potential in Fig. 15.6 shows that an orbit starting out with the particle at rest for $x \to -\infty$ must have $E = 0$. Inserting the explicit potential (15.51) into (15.60), we obtain for $|\phi| < \phi_0$

$$\begin{aligned} x - x_0 &= \pm\frac{2phi_0}{m}\int_0^{\phi}\frac{d\phi'}{(\phi_0-\phi')(\phi'+\phi_0)} = \pm\frac{1}{m}\log\frac{\phi_0+\phi}{\phi_0-\phi} \\ &= \pm\frac{2}{m}\text{artanh}\frac{\phi}{\phi_0}. \end{aligned} \tag{15.61}$$

Thus we find the kink and antikink solution (15.55) crossing the barrier.

The euclidean action of such a solution can be calculated as follows [using (15.58) and (15.59)]:

$$\begin{aligned}\mathcal{A}_{\rm cl} &= \int_{-\infty}^{\infty} dx \left[\frac{{\phi'_{\rm cl}}^2}{2} + V(\phi_{\rm cl}(x))\right] = \int_{-\infty}^{\infty} dx({\phi'}^2_{\rm cl} - E)\\ &= -EL + \int_{-a}^{a} dx\sqrt{2[E+V(\phi)]}. \end{aligned} \tag{15.62}$$

The kink has $E=0$, so that

$$\sqrt{2(E+V(\phi))} = \frac{m}{2\phi_0}(\phi_0^2-\phi^2), \tag{15.63}$$

and the classical action becomes

$$\mathcal{A}_{\rm cl} = \frac{m}{2\phi_0}\int_{-\phi_0}^{\phi_0} d\phi(\phi_0^2-\phi^2) = \frac{2}{3}\phi_0^2 m = \frac{m^3}{3g}. \tag{15.64}$$

Note that for $E=0$, the classical action is also given by the integral

$$\mathcal{A}_{\rm cl} = \int_{-\infty}^{\infty} dx\, \frac{{\phi'_{\rm cl}}^2}{2}. \tag{15.65}$$

There are also solutions starting out at the top of either mountain and sliding down into the adjacent exterior abyss, for instance (see again Fig. 15.6)

$$\begin{aligned} x - x_0 &= \mp\frac{2\phi_0}{m}\int_{\phi}^{\infty}\frac{d\phi'}{(\phi'-\phi_0)(\phi'+\phi_0)} = \pm\frac{1}{m}\log\frac{\phi+\phi_0}{\phi-\phi_0}\\ &= \pm\frac{2}{m}\text{arcoth}\frac{\phi}{\phi_0}. \end{aligned} \tag{15.66}$$

However, these solutions cannot connect the bottoms of the double well with each other and will not be considered further.

The real ϕ^4-theory can be used as a model for a spin system, in which the spins can oint only in two directions. In statistical mechanics, such a system is usually described by the *Ising model* on a lattice. In fact, it can be shown that the Ising model can be transformed into a real ϕ^4-field theory whose potential can be approximated, near the phase transition, by a ϕ^4-potential.[2] The two spin directions are represented in the ϕ^4-theory by the two minima of the potential. The classical solution to the field equation may be interpreted as a domain wall between up and down directions. Domain walls can occur in many possible shapes which are tow hard to calculate analytically. They possess a high configurational entropy, and the demagnetization transition can be understood as a transition in the ensemble of fluctuating domain walls of any shape, whose configurational entropy overcomes the energy it takes to create the domain walls.

Let us finally relaize that domain walls in O(N)-symmetric theories cannot be stable: It is always possible to rotate the domain with one spin direction into the other lowering continuously the energy. This is impossible for a single field ϕ.

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[2] For details see the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, World Scientific, 1989 (http://www.physik.fu-berlin.de/˜kleinert/kleiner_re.html#b1).

15.4 Vortex Lines in O(2)-Symmetric Theory

The most important domain of application of the O(2)-symmetric theory is the physics of the phase transition in superfluid helium at $T_c \approx 2.3\,\mathrm{K}$. The two-component ϕ^4 theory is then referred to as *Landau-Pitajevski theory*. Its euclidean action is written in terms of a complex field $\varphi = (\phi_1 + i\phi_2)/\sqrt{2}$ in 3 space dimensions as an energy density

$$\mathcal{H} = \varphi^*(\mathbf{x}) \left(-\frac{\hbar^2}{2M} \boldsymbol{\nabla}^2 - \mu \right) \varphi(\mathbf{x}) + V |\varphi(\mathbf{x})|^4, \tag{15.67}$$

where μ is the chemical potential which pases through zero at some critical mean-field temperature

$$\mu = \mu_0 \left(\frac{T}{T_c^{\mathrm{MF}}} - 1 \right). \tag{15.68}$$

The quartic term approximates the repulsion between the helium atoms by a δ-function potential [recall the second-quantized Hamiltonian (2.137)]

The field equation which minimizes this energy density is

$$\left(-\frac{\hbar^2}{2M} \boldsymbol{\nabla}^2 - \mu + V|\varphi|^2 \right) \varphi = 0, \tag{15.69}$$

It possesses cylindrical solutions which are observable in the laboratory in the form of straight vortex lines. To find these, we decompose φ into its polar components, $\varphi = \rho e^{i\gamma}$, and find from the real and imaginary parts of (15.69) the two equations

$$\left\{ -\frac{\hbar^2}{2M} \left[\boldsymbol{\nabla}^2 - (\boldsymbol{\nabla}\gamma)^2 \right] - \mu + V\rho^2 \right\} \rho = 0 \tag{15.70}$$

and

$$\boldsymbol{\nabla}(\rho^2 \boldsymbol{\nabla}\gamma) = 0. \tag{15.71}$$

The latter equation is simply the radial-azimuthal form of the current conservation law for the particles

$$\boldsymbol{\nabla}\mathbf{j} = \boldsymbol{\nabla} \left(\frac{1}{2i} \varphi^* \overset{\leftrightarrow}{\boldsymbol{\nabla}} \varphi \right) = 0. \tag{15.72}$$

Equation (15.71) can be solved by a purely circular flow of particles, in which ρ depends on the spatial distance r from the cylindrical axis, and the phase γ of the complex field is an integer multiple of the azimuthal angle in space, $\theta \equiv \tan^{-1}(x_2/x_1)$, i.e.,

$$\gamma = n\theta. \tag{15.73}$$

Then, (15.70) reduces to the radial differential equation

$$-\frac{\hbar^2}{2M} \left(\partial_r^2 + \frac{1}{r} - \frac{n^2}{2} \right) \rho + V(\rho^2 - \rho_0^2)\rho = 0, \tag{15.74}$$

where $\rho_0 = |\varphi_0| = \sqrt{-\mu_0(T/T_c^{\rm MF} - 1)/V}$ [compare (15.68)].

In order to solve Eq. (15.74), it is convenient to go to reduced quantities $\bar{r}, \bar{\rho}$ which measure the distance r in units of the coherence length

$$\xi = \sqrt{2}\xi_{\rm size} = \sqrt{\frac{\hbar^2}{2M}\frac{1}{(-\mu_0)}}\sqrt{\frac{T}{T_c^{\rm MF}} - 1}^{\,-1}, \tag{15.75}$$

and the size of the order parameter ρ in units of ρ_0. Thus we introduce

$$\bar{x} \equiv x/\xi, \qquad \bar{r} \equiv r/\xi, \tag{15.76}$$

in configuration space, and

$$\bar{\rho} = \rho/\rho_0 \tag{15.77}$$

in field space. Then (15.74) takes the form

$$\left[-\left(\partial_{\bar{r}}^2 + \frac{1}{\bar{r}}\partial_{\bar{r}} - \frac{n^2}{\bar{r}^2}\right) + (\bar{\rho}^2 - 1)\right]\bar{\rho}(\bar{r}) = 0. \tag{15.78}$$

For small $\bar{r} \ll 1$, this is dominated by the terms in the first parentheses, leading to a differential equation of the Bessel type for $\bar{\rho}(\bar{r})$. Thus, close to the origin, the solution is

$$\bar{\rho}(\bar{r}) = A_n J_n(\bar{r}) \propto \bar{r}^n, \tag{15.79}$$

where $J_n(\bar{r})$ is the standard Bessel function. Multiplying this with the phase factor

$$e^{in\gamma} = e^{in\tan^{-1}(x_2/x_1)}, \tag{15.80}$$

we see that the complex field $\varphi(x)$ has the following small $|\mathbf{x}|$ behavior

$$\varphi(\mathbf{x}) \propto \bar{r}^n e^{in\tan^{-1}(x_2/x_1)} = (x_1 + ix_2)^n, \tag{15.81}$$

exhibiting a zero of n-th order in the complex plane $x_1 + ix_2$.

For large $\bar{r} \gg 1, \bar{\rho}(\bar{r})$ approaches the asymptotic value $\bar{\rho} = 1$. In fact, from (1.44) we can extract the $1/\bar{r}$ expansion,

$$\bar{\rho}_n(\bar{r}) = 1 - \frac{n^2}{2\bar{r}^2} - \left(n^2 + \frac{1}{8}n^4\right)\frac{1}{\bar{r}^4} - \left(8 + 2n^2 + \frac{1}{16}n^4\right)\frac{n}{\bar{r}^6} - O\left(\frac{1}{\bar{r}^8}\right). \tag{15.82}$$

Integrating the differential equation numerically inward, we find the solution displayed Fig. 15.7. What is the energy of these vortex lines? In order to find a convenient expression for it we use the fact that if $\varphi(\mathbf{x})$ is a solution of the differential equation (15.69), the rescaled solution

$$\varphi_\delta(\mathbf{x}) \equiv e^\delta\, \varphi(\mathbf{x}) \tag{15.83}$$

must extremize the energy inn δ for $\delta = 0$. In terms of the reduced quantities of Eqs. (15.76) and (15.77), the energy is given by

$$E = E_c \int d^3\bar{x} \left[|\boldsymbol{\nabla}\bar{\varphi}|^2 - |\bar{\varphi}|^2 + |\bar{\varphi}|^4\right], \tag{15.84}$$

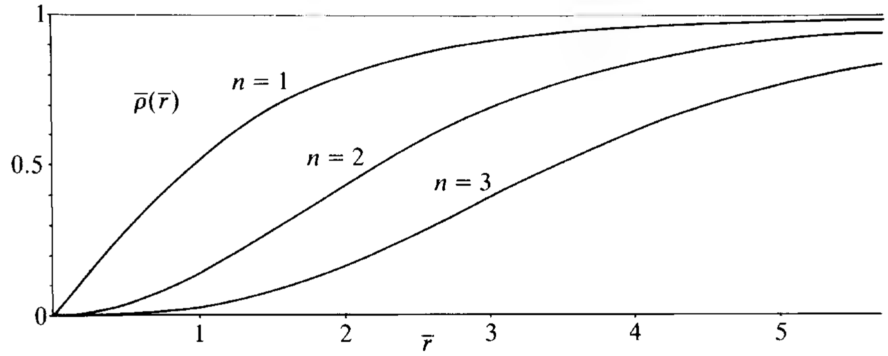

FIGURE 15.7 The order parameter $\bar\rho = |\varphi|/|\varphi_0|$ around a vortex line of strength $n = 1, 2, 3, \dots$ as a function of the reduced distance $\bar r = r/\xi$ where r is the distance from the axis and ξ the healing length.

where

$$E_c = \frac{\mu^2}{4V} \tag{15.85}$$

is the *condensation energy*. Inserting the reduced version of (15.83) into (15.84), we obtain

$$E = E_c \int d^3\bar x \left[e^{2\delta} |\boldsymbol{\nabla} \bar\varphi|^2 - e^{2\delta} |\bar\varphi|^2 + e^{4\delta} |\bar\varphi|^4 \right]. \tag{15.86}$$

Setting the derivative with respect to δ equal to zero gives at $\delta = 0$

$$E_c \int d^3\bar x \left[|\boldsymbol{\nabla}\bar\varphi|^2 - |\bar\varphi|^2 + 2|\bar\varphi|^4 \right] = 0. \tag{15.87}$$

Subtracting this from (15.86) for $\delta = 0$ we find that the energy of a solution of the field equation is simply given by

$$E = -E_c \int d^3\bar x |\bar\varphi|^4. \tag{15.88}$$

Most of this energy is due to the asymptotic value $|\bar\varphi| \to 1$, where E is equal to the negative condensation energy $-E_c$. Subtracting this from E we find the *additioral energy* of the vortex line as

$$E_v = E_c \int d^3 x (1 - |\bar\varphi|^4). \tag{15.89}$$

Going over to cylindrical coordinates $\bar r, \theta, z$, the integral becomes, for a vortex line of length L along the z-direction,

$$E_v = E_c 2\pi \bar L \int_0^{x} d\bar r \bar r \left[1 - \bar\rho^4(\bar r) \right]. \tag{15.90}$$

Before inserting the numerical solutions for $\bar\rho(\bar r)$ shown in Fig. (15.7), we note that due to the factor $\bar r$, the additional energy comes mainly from the large $\bar r$ regime, i.e., from the far zone. In fact, if we insert the leading asymptotic behavior (15.82), we obtain an integral

$$E_v = E_c 4\pi n^2 \bar{L} \int^{\infty} \frac{d\bar{r}}{\bar{r}}, \tag{15.91}$$

which diverges logarithmically for large $\bar{r}$. An immediate conclusion is that a single vortex line can have a finite energy only in a finite container. In a finite cylindrical container of radius R, the integral no longer diverges at the upper end, and we obtain

$$E_v = E_c 4\pi n^2 \bar{L} \log(R/\xi). \tag{15.92}$$

Consider now the energy in the small-$\bar{r}$ regime, where Eq. (15.79) tells us that $\bar{\rho}(\bar{r})$ behaves like $\bar{r}^n$. Hence, $1-\bar{\rho}^4 \approx 1$, and the energy of a thin cylindrical section of radius r grows like r^2. For increasing r, the rate of growth slows down rapidly, and settles at the asymptotic rate $4\pi n^2 L \times \log(\bar{r}/\xi)$, where ξ is the coherence length. The proper inclusion of the non-asymptotic behavior gives simply a finite correction to the asymptotic energy and the energy of a vortex line in a container of radius R becomes

$$E_v = E_c 4\pi n^2 \bar{L}[\log(R/\xi) + c]. \tag{15.93}$$

This is the same result we would have obtained had we replaced in (15.90) the integrand $\bar{r}[1-\bar{\rho}^4(\bar{r})]$ by the asymptotic form $2n^2/\bar{r}$, and integrated from the radius $r_0 = \xi e^{-c}$ to R.

The precise numerical evaluation of the differential equation (15.78) and the integral (15.90) shows that for the lowest vortex line, c has the value

$$c = 0.385. \tag{15.94}$$

Hence the energy of the vortex line becomes

$$E_v = E_c \bar{L} 4\pi n^2 [\log(R/\xi) + 0.385]. \tag{15.95}$$

The logarithmic divergence of the energy has a simple physical origin. In order to see this let us calculate the energy once more in another way, using the original expression (15.84), i.e. without invoking the virial theorem. It reads, for the radial solutions,

$$E_v = E_c 4\pi \bar{L} \int d\bar{r}\bar{r} \left[(\partial_{\bar{r}}\bar{\rho})^2 + \frac{1}{2}(1-\bar{\rho}^2)^2 + \frac{n^2}{\bar{r}^2}\bar{\rho}^2 \right]. \tag{15.96}$$

The first two terms are rapidly convergent. Thus the energy of the far zone resides completely in the last term

$$\frac{n^2}{\bar{r}^2}\bar{\rho}^2 \approx \frac{n^2}{\bar{r}^2}. \tag{15.97}$$

This energy is a consequence of the angular behavior of the condensate phase $\gamma = n\tan^{-1}(x_2/x_1)$ around a vortex line. It comes entirely from the *azimuthal part* of the gradient energy $(\hbar^2/2M^2)|\varphi|^2(\boldsymbol{\nabla}\gamma)^2$, i.e., the term which describes the *Nambu-Goldstone modes.* This is not surprising. We have discussed before that the *long range properties* of the system are dominated by these modes. A phase of the field φ which behaves like $\gamma = n\tan^{-1}(x_2/x_1)$ can be viewed as a coherent pile-up of these modes determining the energy in the far zone.

The dominance of the energy carried by the phase gradient can also be described in a different and more physical way. In the last section we identified the gradient $(\hbar/M)\boldsymbol{\nabla}\gamma$ with the superfiuid velocity. For the vortex line at hand, the superfiuid velocity is found, far away from the line, to be

$$\mathbf{v}_s = \frac{\hbar}{M}n\boldsymbol{\nabla}\tan^{-1}\left(\frac{x_2}{x_1}\right) = \frac{\hbar}{M}\frac{n}{r^2}(-x_2, x_1, 0) = \frac{\hbar}{M}n\frac{1}{r}\mathbf{e}\phi, \tag{15.98}$$

where $\mathbf{e}_\phi$ is the unit vector in azimuthal direction. Thus, around every vortex line, there is a circular fiow of the superfiuid whose velocity decreases like the inverse distance from the line. The hydrodynamic energy density of this flow is

$$e(\mathbf{x}) = \frac{\rho_s}{2}\mathbf{v}_s^2 = \frac{\rho_s}{2}\frac{\hbar^2}{M^2}\frac{n^2}{r^2}. \tag{15.99}$$

This is precisely the dominant third Nambu-Goldstone term in the energy integral (15.96). Thus the energy of the vortex line is indeed mainly due to the hydrodynamic energy of the superfiow around the line. For the major part of the volume, the hydrodynamic limit (15.98), (15.99) gives an excellent approximation. Only in the neighborhood of the line, i.e., for small radii $r \leq \xi$, the energy density differs from (15.99) due to gradients in the size of the field $|\varphi|$. It is therefore suggestive to idealize the superfiuid and assume the validity of the pure gradient energy density

$$\varepsilon = \frac{\rho_s}{2}\mathbf{v}_s^2 = \frac{\sigma}{2}(\boldsymbol{\nabla}\gamma)^2, \quad \sigma \equiv \rho_s\frac{\hbar^2}{M^2}, \tag{15.100}$$

everywhere in space, where ρ_s is the *superfluid density.*

The deviations from this law, which become significant only very clnse to a vortex line, i.e., at distances of the order of the coherence length ξ, are treated approximately by simply cutting off the energy integration at a radius ξ away from a vortex line. In other words, we pretend as though there were no superflow at all within the thin tubes of radius ξ, with a sudden onset of idealized flow outside ξ, moving with the limiting velocity (15.98).

Although the internal part of the thin tube carries no superfiow, it nevertheless carries rotational energy. Within the present approximation, this energy is associated with the number 0.385 in (15.95). This piece will be called the *core energy.* The core enrgy has a physical interpretation. At distances smaller than the coherence length, the different parts of the liquid can no longer slip past each other freely.

Hence the core of a vortex line is expected to rotate roughly like a solid rod, rather than with the diverging velocity $\nu_s \sim 1/r$. Indeed, if we use the approximation

$$\nu_s \propto n \begin{cases} \dfrac{1}{r}, & r > \xi, \\ \dfrac{r}{\xi^2}, & r \leq \xi, \end{cases} \tag{15.101}$$

for a line of vortex strength n, the energy density does behave like r^2, for small r, as observed before. Moreover, the energy integration gives

$$n^2 \left[\int_1^{R/\xi} d\bar{r}/\bar{r} + \int_0^1 d\bar{r}\bar{r}^3 \right] = n^2 [\log(R/\xi) + 0.25], \tag{15.102}$$

and we see that the number for the core energy, 0.25, emerges with the right order of magnitude. We complete our discussion of the hydrodynamic picture, let us calculate the circulation of the superftuid velocity field around the vortex lines:

$$\kappa \equiv \oint_B d\mathbf{x} \cdot \mathbf{v}_s = \frac{\hbar}{M} n \oint_B d\mathbf{x} \cdot \boldsymbol{\nabla}\gamma = \frac{\hbar}{M} 2\pi n = n \frac{h}{M} = n\kappa_1. \tag{15.103}$$

This integral is the same for any size and shape of the circuit B around the vortex line. Thus the circulation is quantized and always appears in multiplets of $\kappa_1 = h/M \approx 10^{-3}$ cm^2/sec. The number n is called *vortex strength* .

The integral (15.103) can be transformed into a surface integral, via Stokes' theorem:

$$\int_{S^B} d\mathbf{S} \cdot (\boldsymbol{\nabla} \times \mathbf{v}_s) = \frac{\hbar}{M} 2\pi n, \tag{15.104}$$

where S^B is some surface spanned by the circuit B in (15.103), and $d\mathbf{S}$ is the surface element. This integral is the same for any size and shape of S^B. From this result we conclude that the third component of the curl of $\mathbf{v}_s$, must vanish everywhere except at the origin. There it must have a singularity of such a strength that the two-dimensional integral gives the correct vortex strength. Hence

$$\boldsymbol{\nabla} \times \mathbf{v}_s = \frac{\hbar}{M} 2\pi n \delta^{(2)}(\mathbf{x}_T)\hat{\mathbf{z}}, \tag{15.105}$$

where $\hat{\mathbf{z}}$ is the unit vector along the z-axis and $\mathbf{x}_T \equiv (x_1, x_2)$ are the coordinates orthogonal to the vortex line.

If the nonlinearities of the field equation are taken into account, the $\delta^{(2)}$-function is really smeared out over a circle whose radius is of order ξ. As an example, let us replace $1/r^2$ in (15.99) by $1/(r^2 + \varepsilon^2)$. Then the rotation of the superftuid velocity becomes

$$\boldsymbol{\nabla} \times \mathbf{v}_s = \frac{\hbar}{M} n \frac{2\varepsilon^2}{(r^2 + \varepsilon^2)^2} \hat{\mathbf{z}}. \tag{15.106}$$

The right-hand side is non-zero only within a small radius $r \neq \varepsilon$, where it diverges with the total strength

$$\int d^2x \frac{2\varepsilon^2}{(r^2+\varepsilon^2)^2} = 2\pi\varepsilon^2 \int_0^\infty dr \frac{2r}{(r^2+\varepsilon^2)^2} = 2\pi. \tag{15.107}$$

This shows that (15.106) is, indeed, a smeared out version of the δ-function relation (15.105).

Because of their rotational properties, vortex lines can be generated experimentally by rotating a vessel with an angular velocity m. Initially, the lack of friction will cause the superfluid part of the liquid to remain at rest. This situation cannot, however, persist forever since it is not in a state of thermal equilibrium. After some time, vortex lines form on the walls which migrate into the liquid and distribute evenly. This goes on until their total number is such that the rotational Helmholtz free energy

$$F_\Omega = F - \Omega \cdot \mathbf{L} \approx \int d^3x \left(\frac{\rho_s}{2} \mathbf{v}_s^2 - \Omega \cdot \mathbf{x} \times \rho_s \mathbf{v}_s \right) \tag{15.108}$$

is minimal. This equilibration process has been observed in the laboratory and has even been photographed directly using the property that vortex lines trap ions which can be accelerated against a photographic plate. Integrating (15.108) with $\mathbf{v}_s$ from (15.98), we find that in a cylindrical vessel of radius R, the first vortex line $n = 1$ appears at a critical angular velocity

$$\Omega_c = \frac{\kappa_1}{\pi R^2} \log \frac{R}{\xi} \tag{15.109}$$

and settles on the axis of rotation. It is useful to observe that the vortex lines of higher n are all unstable. Since the energy increases quadratically with n, it is favorable for a single line of higher n to decay into n lines of unit strength each. When generating vortex lines by stirring a vessel, one may nevertheless be able to create, for a short time, such an unstable line, and to observe its decay.

16

Scalar Quantum Electrodynamics

In nature, there also exist charged scalar particles which are coupled to the electromagnetic field. In three spatial dimensions, a historic example which supplied many important predictions of experimental data is the *Ginzburg-Landau theory* of superconductivity. The generalization of this theory to four spacetime dimensions is of great importance in elementary particle physics, where it is known as *scalar quantum electrodanymics* (scalar QED).

16.1 Action and Generating Functional

The Ginzburg-landau theory is a three-dimensional euclidean quantum field theory containing a a complex scalar field

$$\varphi(\mathbf{x}) = \varphi_1(\mathbf{x}) + i\varphi_2(\mathbf{x}) \tag{16.1}$$

coupled to a magnetic vector potential $\mathbf{A}$. The scalar field describes bound states of pairs of electrons, which arise in a superconductor at low temperatures due to an attraction coming from elastic forces. The detailed mechanism will not be of interest her; we only note that the pairs are bound in an S-wave and a spin singlet state of charage $q = 2e$. Ignoring for a moment the magnetic interactions, the ensemble of these bound states may be described in the neighborhood of the superconductive transition temperature T_c by a complex scalar field theory of the φ^4 type, with a euclidean action

$$\mathcal{A}_E = \int d^3x \left[\frac{1}{2}\boldsymbol{\nabla}\varphi^*\boldsymbol{\nabla}\varphi + \frac{m^2}{2}\varphi^*\varphi + \frac{g}{4}\left(\varphi^*\varphi\right)^2\right]. \tag{16.2}$$

The mass parameter depends on the temperature like $m^2 \propto (T - T_c)/T_c$. Above the transition temperature, the parameter m^2 is positive, below it is negative. As a consequance, the system exhibit a spontaneous symmetry breakdown discussed in Chapter 15. The symmetry group which is broken is the U(1)-symmetry

$$\varphi(x) \to e^{-i\alpha}\varphi(x) \tag{16.3}$$

under which $\mathcal{A}_E$ is obviously invariant. Alternatively we may write

$$\begin{aligned} \varphi_1 &\rightarrow \quad \cos\alpha\,\varphi_1 + \sin\alpha\,\varphi_2 \\ \varphi_2 &\rightarrow -\sin\alpha\,\varphi_1 + \cos\alpha\,\varphi_2 \end{aligned} \tag{16.4}$$

so that we may equally well speak of a broken O(2)-symmetry.

The action (16.2) is the euclidean version of a relativistic field theory in $D = 1{+}2$ dimensions with an action

$$\mathcal{A} = \int d^D x \left[\frac{1}{2}\partial_\mu\varphi^*\partial^\mu\varphi - \frac{m^2}{2}\varphi^*\varphi - \frac{g}{4}\left(\varphi^*\varphi\right)^2\right]. \tag{16.5}$$

For the sake of generality, we shall discuss this theory for arbitrary D. Most formulas will be written down explicitly in $D = 4$ dimensions, to emphasize analogies with proper QED in Chapter 10.

The phenomenon of spontaneous symmtry breaking in this system has been studied in detail in Chapter 15. For $T > T_c$, where the mass term is positive, small oscillations around $\varphi = 0$ consist of two degenerate modes carried by φ_1, φ_2, both of mass m^2. For $T < T_c$, where the mass is negative, the energy is minimized by a field φ with a non-vanishing vacuum expectation value, say

$$\langle\varphi(\mathbf{x})\rangle \equiv (\phi_0, 0). \tag{16.6}$$

Then the symmetry between φ_1 and φ_2 is broken and there are two different modes of small oscillations: one orthogonal to $\langle\varphi\rangle$ which is the massless Nambu-Goldstone mode, and one parallel to $\langle\varphi\rangle$ which has a positive mass $-2m^2 > 0$.

In order for the euclidean version of (16.5) to describe the phenomena of superconductivity, we must include electromagnetism. According to the minimal substitution rules described in Chapter 10, we simply replace $\partial_\mu\varphi$ in (16.5) by the covariant derivative

$$\partial_\mu\varphi \rightarrow \left(\partial_\mu - iqA_\mu\right)\varphi, \tag{16.7}$$

and add the free electromagnetic action[1]

$$\mathcal{A}_\gamma = -\int d^D x \frac{1}{4} {F_{\mu\nu}}^2. \tag{16.8}$$

The combined action becomes

$$\mathcal{A} = \int d^D x \left\{\frac{1}{2}|D_\mu\varphi|^2 - \frac{m^2}{2}|\varphi|^2 - \frac{g}{4}|\varphi|^4 - \frac{1}{4}{F_{\mu\nu}}^2\right\}. \tag{16.9}$$

This action is invariant under local gauge transformations

$$\varphi(x) \rightarrow e^{iq\Lambda(x)}\varphi(x), \qquad A_\mu(x) \rightarrow A_\mu(x) + \partial_\mu\Lambda(x). \tag{16.10}$$

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[1] In this chapter we use natural units with $\hbar = c = 1$.

The generating functional is given by the functional integral

$$Z\left[\lambda,\lambda^*,j\right] = \int \mathcal{D}\varphi\mathcal{D}\varphi^* \int_{\rm phys.} \mathcal{D}A^\mu e^{i\{\mathcal{A}[\varphi,\varphi^*]+i\mathcal{A}_{\rm s}[\varphi,\varphi^*,A;\lambda,\lambda^*,j]\}}, \tag{16.11}$$

where

$$\mathcal{A}_{\rm s}[\varphi,\varphi^*,A;\lambda,\lambda*,j] \equiv -\lambda^*\varphi-\varphi^*\lambda-j^\mu A_\mu \tag{16.12}$$

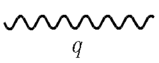
collects the sources $\lambda(x)$, $\lambda^*(x)$ for the complex scalar fields $\varphi^*(x)$ and $\varphi(x)$, and j^μ is the usual electromagnetic current, the latter being a conserved quantity with $\partial_\mu j^\mu(x)=0$. The path integral $\int_{\rm phys.}\mathcal{D}A^\mu$ infdicates that a Fadeev-Popov gauge fixing factor is inserted, together with a compensating determinant (recall the general discussion in Section 10.10):

$$\int_{\rm phys.} \mathcal{D}A^\mu \equiv \int \mathcal{D}A^\mu \Phi^{-1}[A]F[A]. \tag{16.13}$$

For $m^2>0$, we may choose [recall (10.170)]

$$F[A]=F_4[A]=e^{-\frac{1}{2\alpha}(\partial_\mu A^\mu)^2}, \tag{16.14}$$

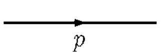
and derive from it Feynman rules for perturbation expansions. with a photon propagator (10.190):



$$G_{0\,\mu\nu}(x-y) = -\int \frac{d^Dk}{(2\pi)^D} e^{-ik(x-y)} \frac{i}{k^2}\left[g_{\mu\nu}-(1-\alpha)\frac{k_\mu k_\nu}{k^2}\right]. \tag{16.15}$$

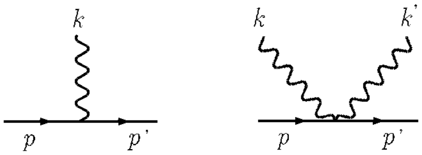
We have seen in Chapter 10 that in QED all scattering amplitudes are independent of of the gauge parameter α.

In addition, the pertubation expansion associated with the action (16.12) involves propagators of scalar particles



$$e^{-ik(x-y)} \qquad G_0(x-y) = \int \frac{d^Dk}{(2\pi)^D} e^{-ik(x-y)} \frac{i}{k^2} \tag{16.16}$$

and vertices



(16.17)

Since the scalar field is complex, the particle carries a charge and the line in the Feynman diagram an orietation. The coupling of the scalar field to the vector potential gives not only rise to a three-vertex analog to (10.89) in QED, but also to a four vertex in which two photons are absorbed or emitted by a scalar particle. This diagram is commonly referred to as *seagull diagram*.

16.2 Meissner-Higgs Effect

The situation is drastically different for $T < T_c$ where $m^2 < 0$. At the classical level, the lowest energy state of the pure φ theory is reached if $|\varphi| = \phi_0 = \sqrt{-m^2/g}$, say

$$\varphi = \phi_0 e^{-i\gamma_0} = \sqrt{\frac{-m^2}{g}} e^{-i\gamma_0}. \tag{16.18}$$

Inserting this into the action (16.12), its photon part becomes

$$\mathcal{A}_\gamma = \int d^D x \left(-\frac{1}{4} F_{\mu\nu}^2 - \frac{q^2}{2} \frac{m^2}{g} A_\mu{}^2 \right). \tag{16.19}$$

Extremizing this gives the Euler-Lagrange equation

$$\partial^2 A_\mu - \partial_\mu \partial A = \frac{q^2 m^2}{g} A_\mu = 0. \tag{16.20}$$

Note that we could have chosen as well

$$\varphi = \phi_0 e^{-i\gamma_0(x)} = \sqrt{\frac{-m^2}{q}} e^{-i\gamma_0(x)}, \tag{16.21}$$

with an arbitrary spacetime-dependent phase $\gamma_0(\mathbf{x})$. Then the photon Lagrangian would read

$$\mathcal{A}_\gamma = \int d^D x \left[-\frac{1}{4} F_{\mu\nu}^2 - \frac{q^2}{2} \frac{m^2}{g} \left(A_\mu - \partial_\mu \gamma_0 \right)^2 \right]. \tag{16.22}$$

with Euler Lagrange equations

$$\partial^2 A_\mu - \partial_\mu (\partial A) - q^2 \frac{m^2}{g} \left(A_\mu - \partial_\mu \gamma_0 \right) = 0 \tag{16.23}$$

and the minimal energy would be reached for

$$A_\mu(x) = \partial_\mu \gamma_0(x). \tag{16.24}$$

Of course, the two results are equivalent by a gauge transformation $A_\mu \to A_\mu + \partial_\mu \gamma_0(x)$ and their physical content is independent on the particular choice of $\gamma_0(x)$.

Consider now the fluctuation properties of this theory. The generating functional has the form (16.11) in which the measure sums over all φ and physical A^μ configurations orthogonal to the gauge degrees of freedom. If we decompose φ into radial and azimuthal parts

$$\varphi(x) = \rho(x) e^{-i\gamma(x)} \tag{16.25}$$

the path integral takes the form

$$Z\left[\lambda,\lambda^*,j\right]=\int\rho\mathcal{D}\rho\mathcal{D}\gamma\int_{\text{phys}}\mathcal{D}Ae^{i\mathcal{A}[\varphi_1 A_\mu]+i\mathcal{A}_{\rm s}[\varphi,\varphi^*,A;\lambda,\lambda^*,j]}. \tag{16.26}$$

But from the structure of the covariant derivative it is obvious that no matter what the fluctuating $\gamma(x)$ configuration is, it can be absorbed into $A(x)$ as a longitudinal degree of freedom. Thus we have the option of considering complex fields $\varphi(x)$ together with physical, transverse, A^μ fluctuations, or real ρ together with transverse *and* longitudinal $A^\mu(x)$-fluctuations. This may be expressed by rewriting the functional integral (16.26) as

$$Z\left[\lambda,\lambda^*,j\right]=\int\rho\mathcal{D}\rho\int_{\text{all}}\mathcal{D}A^\mu e^{i\mathcal{A}[\rho,A_\mu]+i\mathcal{A}_{\rm s}[\varphi,\varphi^*,A;\lambda,\lambda^*,j]}, \tag{16.27}$$

with the action

$$\mathcal{A}[\rho,A_\mu]=\int d^Dx\left[\frac{1}{2}\left(\partial_\mu\rho\right)^2+\frac{q^2}{2}\rho^2{A_\mu}^2-\frac{m^2}{2}\rho^2-\frac{g}{4}\rho^4+\frac{1}{4}{F_{\mu\nu}}^2\right]. \tag{16.28}$$

The formerly irrelevant gauge degree of freedom in $A^\mu(x)$ has now become a physical one, accounting for the phase oscillations of the complex φ-field.

Let us describe the situation more precisely in terms of a gauge-fixing functional $F[A]$ of (10.13) and a compensating Fadeev-Popov determinant $\Phi^{-1}[A]$. expression (10.172). Whereas all former gauge consitions involved only the $A^\mu(x)$-field itself, this is no longer true here. Since the transformations of A_μ and φ are coupled, the gauge condition may involve both fields (or any other field) of the system. Here

$$F[A_\mu,\varphi]=0, \tag{16.29}$$

to be compensated by a functional $\Phi[A_\mu,\varphi]$, which also depends on both fields. The latter is determined by the integral over the gauge volume as in (10.172):

$$\Phi[A_\mu,\varphi]=\int\mathcal{D}\Lambda F\left[A^\Lambda,\varphi^\Lambda\right]. \tag{16.30}$$

The above discussion corresponds to choosing a gauge condition which ensures the reality of the complex scalar field φ via the δ functional:

$$F[A_\mu,\varphi]=\delta[\varphi_2(x)]. \tag{16.31}$$

where $\varphi_2(\mathbf{x})=\text{Im}\varphi(\mathbf{x})$. Since the gauge transformations change

$$\varphi\rightarrow e^{-i\Lambda(x)}\varphi=\left[\cos\Lambda(x)\,\varphi_1+\sin\Lambda(x)\,\varphi_2\right]+i\left[-\sin\Lambda(x)\,\varphi_1+\cos\Lambda(x)\varphi_2\right], \tag{16.32}$$

we see that

$$\Phi[A_\mu,\varphi]=\int\mathcal{D}\Lambda\,\delta\left[-\sin\Lambda\,\varphi_1+\cos\Lambda\,\varphi_2\right]. \tag{16.33}$$

The result must be independent of the choice of gauge and can therefore be obtained at $\varphi = (|\varphi|, 0)$ where we find

$$\Phi[A_\mu, \varphi] = \frac{1}{|\varphi(x)|}. \tag{16.34}$$

Note that Φ involves no derivative terms as in the eaarlier gauges. For this reason it does not require Fadeev-Popov ghost fields. Setting $\varphi = \rho(x)e^{-i\gamma(x)}$ we arrive precisely at the functional integral (16.28). The Faddev-Popov determinant $\Phi_{-1} = \rho(x)$ turns out to be responsible for give the integral at each point a form expected from the radial-azimutzal decomposition $\varphi = \rho e^{-i\gamma}$ and the accociated integration measure $d\varphi d\varphi^* = d\varphi_1 d\varphi_4 = \rho d\rho d\gamma$.

The generating functional (16.27) may now be used for perturbation expansions below T_c. Inserting into (16.28)

$$\rho(x) = \rho_0 + \rho'(x) = \sqrt{-\frac{m^2}{g}} + \rho'(x) \tag{16.35}$$

we can rewrite

$$\begin{aligned} \mathcal{A} = \int d^D x \Bigg[& \frac{1}{2}\left(\partial_\mu \rho'\right)^2 - \frac{(-2m^2)}{2}\rho'^2 - \frac{g}{4}\rho'^4 - \frac{3}{2} g\rho_0\rho'^3 \\ & -\frac{1}{4}F_{\mu\nu}{}^2 + \frac{\mu^2}{2} + A_\mu^2 q^2 \rho_0 \rho' A_\mu 2 + \frac{q^2}{2}\rho'^2 A_\mu{}^2 \Bigg]. \end{aligned} \tag{16.36}$$

with $\mu^2 \equiv -qm^2/g$. From the quadratic part in ρ' we can deduce the massive ρ' propagator

$$\rho'(x)\rho'(0) = \int \frac{dq}{(2\pi)^4} e^{-iqx} \frac{i}{q^2 - (-2m^2) + i\eta}. \tag{16.37}$$

the ρ' field has cubic ρ'^3 and quadratic ρ'^4 interactions. In addition there are the elcetromagnetic vertices in which one or two particle couple to two photons

$$q^2 \rho_0 \tag{16.38}$$

The most important new feature is found in the propagator of the photon field. If we the quadratic photon part of the action in momentum space it becomes

$$\mathcal{A} = -\frac{1}{2}\int \frac{dk}{(2\pi)^4} A_\mu(-k)\left[k^\mu k^\nu - g^{\mu\nu}\left(k^2 - \mu^2\right)\right] A_\nu(k) \tag{16.39}$$

we can immediately form the inverse of

$$\begin{aligned} M^{\mu\nu} &= k^\mu k^\nu - g^{\mu\nu}\left(k^2 - \mu^2\right) && (16.40) \\ &= -\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2}\right)\left(k^2 - \mu^2\right) + \mu^2 \frac{k^\mu k^\nu}{k^2} && (16.41) \end{aligned}$$

as

$$M^{-1}_{\mu\nu} = -\frac{g^{\mu\nu} - k^\mu k^\nu/k^2}{k^2 - \mu^2} + \frac{1}{\mu^2}\frac{k^\mu k^\nu}{k^2} = -\frac{g^{\mu\nu} - k^\mu k^\nu/\mu^2}{k^2 - \mu^2} \tag{16.42}$$

such that the massive propagator becomes

$$G_{\mu\nu}(x) = \int \frac{dk}{(2\pi)^4} e^{-ikx} \frac{-i}{k^2 - \mu^2}\left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right). \tag{16.43}$$

The photon has acquired a mass and can no longer propagate over a long range. the dramatic experimental consequence is known as the Meißner effect: If a superconductor is cooled below T_c, the magnetic field lines are expelled and can invade only a thin surface layer of penetration depth $1/\mu$.

At $k^2 = \mu^2$ there is a massive particle pole. Since at this place, the propagator $G_{\mu\nu}(x)$ is purely transverse, it satisfies

$$k^\mu G_{\mu\nu}(k) = 0, \tag{16.44}$$

and these particles have three internal degrees of freedom corresponding to a massive particles of unit spin. This is to be contrasted to the massless gauge invariant theory for $T > T_c$ where gauge invariance permits to choose, say, $A^0 = 0$ while still satisfying (16.44) at the pole , thereby eliminating one more degree of freedom in the asymptotic states. Only two transverse photon polarizations remain far away from the interaction. There is no contradiction in the number of degrees of freedom since for $T > T_c$ there are two modes carried by the complex φ fields. The third photon degree is a consequence of absorbing into the vector field the phase oscillations, i.e., the former Nambu-Goldstone degrees of freedom. One sometimes describes this process by saying: The photon has "eaten up" the would-be Nambu-Goldstone boson and has grown fat and massive.

Certainly, the same theory can also be calculated with the earlier gauge fixing Lagnranian

$$\mathcal{L}_{\rm GF} = -\frac{1}{2\alpha}\left(\partial^\mu A_\mu\right)^2, \tag{16.45}$$

in which case the quadratic piece of the action is

$$\mathcal{A}^{\rm quad} = \int d^D x \left[\frac{1}{2}\left(\partial_\mu \rho'\right)^2 - \frac{\left(-2m^2\right)}{2}\rho'^2 \right. \tag{16.46}$$
$$\left. -\frac{1}{4}{F_{\mu\nu}}^2 + \frac{\mu^2}{2}\left(A_\mu - \frac{1}{q}\partial_\mu \gamma\right)^2 - \frac{1}{2\alpha}\left(\partial_\mu A^\mu\right)^2\right].$$

Recalling the Faddev-Popov determinant Φ_4^{-1} of (10.182), for this gauge we have to add the Fadeev-Popov ghost action corresponding ton (10.226):

$$\mathcal{A}_{\rm ghost} = -\frac{1}{2\alpha}\partial_\mu c^* \partial^\mu c \tag{16.47}$$

to complete the list of fluctuating fields present in this gauge.

The generating functional is obtained by integrating $e^{i\mathcal{A}}$ over all $A_\mu(x)$, all complex $\varphi(x)$, and all ghost configurations $c^*(x), c(x)$:

$$Z\left[\lambda, \lambda^*, j\right] = \int \mathcal{D}c\mathcal{D}c^* \int \mathcal{D}\varphi\mathcal{D}\varphi^* \int \mathcal{D}Ae^{i\mathcal{A}}. \tag{16.48}$$

What is the particle content of this theory? Since the Fadeev-Popov ghosts do not interact witgh the other particles, they can be ignored. As far as the photon field is concerned, let us split the vecter potential a

$$A_\mu = A^t_\mu + A^l_\mu \tag{16.49}$$

where A^t is the transverse part satisfying the Lorentz gauge condition $\partial^\mu A^t_\mu = 0$, and A^l is the longitudinal part $A^l_\mu = \partial^{-2}\partial_\mu\partial_\nu A^\nu$, which is a pure gauge.[2] Then the Lorentz part is diagonal and has the propagator

$$\dot{A}^t_\mu(x)\dot{A}^t_\nu(0) = \int \frac{dk}{(2\pi)^4}\frac{-i}{k^2-\mu^2}\left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right). \tag{16.50}$$

The gauge-like pieces, on the other hand, are coupled with the would-be Nambu-Goldstone mode. In terms of $A_\mu = k_\mu\Lambda, \gamma' \equiv \frac{1}{q}\gamma$ we find the quadratic action

$$\frac{\mu^2}{2}(\Lambda\gamma')\begin{pmatrix} k^2-\alpha^{-1}k^4 & -k^2 \\ -k^2 & k^2 \end{pmatrix}\begin{pmatrix} \Lambda \\ \gamma' \end{pmatrix} \tag{16.51}$$

which has the determinant $-\mu^4/4\alpha k^6$ and eigenvalues

$$\lambda_k = \frac{\mu^2 k^2}{2}\left[1 - \frac{1}{2\alpha}\frac{k^2}{\mu^2} \pm \sqrt{1+\left(\frac{k^2}{2\alpha\mu^2}\right)^2}\right] \tag{16.52}$$

which both vanish at $k^2 = 0$ (and only there). Thus there are two more massless asymptotic states in the Hilbert space. At first sight, this formulation describes a physical situation different from the previous one. We do know, however, that the generating functionals are the same. In the previous formulation, there were only two types of particles. Therefore all the additional zero mass asymptotic states found in the present gauge must be such that if a scattering process takes place with the two physical particles coming in, the unphysical ones can never be produced. Physical and unphysical states should have no mutual interaction. We may say that the S-matrix is irreducible on the set of physical states. For the Fadeev-Popov ghost fields this is trivial to see. With respect to the other states, however, it is not and the path integral is the only efficient tool for convincing us of the correctness of this statement as we demonstrated in Section 10.10. The irreducibility of the

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[2] As in (10.187), the letters l and t stand for longitudinal and transverse to the *four*-vector field $A_\mu(x)$.

S-matrix becomes most transparent by using a particular gauge due to t'Hooft in which physical and unphysical parts of the Hilbert space receive a clear distinction which depends on the gauge parameter. Consider the gauge condition

$$F\left[A,\varphi\right]=\exp\left[-\frac{1}{2\alpha}\left(\partial_\mu A^\mu-\frac{\mu^2}{q}\alpha\gamma\right)^2\right]. \tag{16.53}$$

For $\alpha\longrightarrow 0$ this enforces the Lorentz gauge. The exponent has the pleasant advantage that when added to the free part of the Lagrangian, the term which mixes γ with the gauge-like component of A_{μ_1} and which requires diagonalization in (16.51), cancels. Therefore, barring the calculation of $\Phi[A,\varphi]^{-1}$, gauge-fixed free action reads

$$\begin{aligned}\mathcal{A}^{\text{free}}=\int d^Dx\left\{\frac{1}{2}\left(\partial\rho'\right)^2-\frac{-2m^2}{2}\rho'^2-\frac{1}{4}F_{\mu\nu}{}^2+\frac{\mu^2}{2}A_\mu^2\right.\\ \left.+\frac{\mu^2}{2q^2}\left[\left(\partial_\mu\gamma\right)^2-\alpha\mu^2\gamma^2\right]-\frac{1}{2\alpha}\left(\partial_\mu A^\mu\right)^2\right\}.\end{aligned} \tag{16.54}$$

Thus the photon has a quadratic piece

$$\begin{aligned}&\frac{1}{2}A^\mu(-k)\left[-\left(k^2-\mu^2\right)q_{\mu\nu}+k_\mu k_\nu-\frac{1}{\alpha}k_\mu k_\nu\right]A^\nu(k)\\ &=\frac{1}{2}A^\mu(-k)\left[-\left(k^2-\mu^2\right)\left(q_{\mu\nu}-\frac{k_\mu k_\nu}{k^2}\right)-\frac{k^2-\alpha\mu^2}{\alpha}\frac{k^\mu k^\nu}{k^2}\right]A^\nu(k),\end{aligned} \tag{16.55}$$

whose inversion leads to a propagator

$$G_{\mu\nu}(x)=\int\frac{dk}{(2\pi)^4}e^{-ikx}\left[-\frac{i}{k^2-\mu^2}\left(g_{\mu\nu}-\frac{k_\mu k_\nu}{k^2}\right)-\frac{i\alpha}{k^2-\alpha\mu^2}\frac{k^\mu k^\nu}{k^2}\right]. \tag{16.56}$$

Apart from the physical propagator, there is a ghost-like state in $A^\mu(k)$ proportional to k^μ.

The new feature of this gauge is that the would-be Nambu-Goldstone mode $\gamma(x)$ has acquired a mass term $\alpha\mu^2\gamma^2(x)$. The reason for this lies in the fact that the gauge fixing term destroys explicitly also the global invariance of the Lagrangian

$$\varphi(x)\longrightarrow e^{-i\Lambda}\varphi(x),\qquad \gamma(x)\longrightarrow\gamma(x)+\Lambda,\qquad A_\mu\longrightarrow A_\mu, \tag{16.57}$$

under which the gauge pieces transform as

$$-\frac{1}{2\alpha}\left(\partial_\mu A^\mu-\frac{\mu^2}{q}\alpha\gamma\right)^2\longrightarrow-\frac{1}{2\alpha}\left[\partial_\mu A^\mu-\frac{\mu^2}{q}\alpha(\gamma+\Lambda)^2\right]. \tag{16.58}$$

Therefore, pure phase transformations change the energy and this results in a mass term.

Let us now take a look at the functional $\Phi[A,\varphi]$ in order to see that this does not modify the Lagrangian (16.54). According to (10.172), we have to integrate

$$\begin{aligned}\Phi[A,\varphi] &= \int\mathcal{D}\Lambda\exp\left[-\frac{1}{2\alpha}\left(\partial^\mu A^\Lambda_\mu-\frac{\mu^2}{q}\alpha\gamma\Lambda\right)^2\right]\\ &= \int\mathcal{D}\Lambda\exp\left[-\frac{1}{2\alpha}\left(\partial^\mu A_\mu+\partial^2\Lambda-\frac{\mu^2_\alpha}{q}(\gamma+\Lambda)\right)^2\right] \qquad (16.59)\\ &= \int\mathcal{D}\Lambda\exp\left[-\frac{1}{2\alpha}\left(\partial^\mu A_\mu-\frac{\mu^2}{q}\alpha\gamma+\left(\partial^2-\frac{\mu^2}{q}\alpha\right)\Lambda\right)^2\right]\end{aligned}$$

which after a shift of the integration variable gives the trivial constant

$$\Phi[A,\varphi]=\det\left(-\partial^2+\frac{\mu^2}{q}\alpha\right)/\sqrt{\alpha}. \tag{16.60}$$

This can be expressed in terms of Fadeev-Popov ghost fields as

$$\Phi^{-1}[A,\varphi]=\int\mathcal{D}c\mathcal{D}c^*\exp\left[\frac{i}{\sqrt{\alpha}}\int dx\left(\partial c^*\partial c+\frac{\mu^2}{q}\alpha c^*c\right)\right]. \tag{16.61}$$

The situation is similar to that of the last gauge condition: There are three additional kinds of asymptotic states: Fadeev-Popov ghosts, ghost-like poles in the gauge part of the photon field and a state carried by the would-be Nambu-Goldstone field. But contrary to the previous case. all these states now have a mass which depends on the gauge parameter α. This proves that they must be artifacts of the gauge choice and cannot contribute to physical processes. In particular, by letting the parameter α tend to infinity, all these particles become infinitely heavy and are thus eliminated from the physical Hilbert space.

16.3 Spatially Varying Ground States

The theory of a complex scalar field interacting with a photon has another interesting feature. The ground state must not necessarily be uniform. There are ranges of mass, and external source where the system prefers to be filled with string like field configurations and others where the fields have spatially periodic structure of the hexagonal type. In order to see how this comes about and to be able to compare results with experimental data we consoder the euclidean three-dimensiona scalar QED, which is the *Ginzburg-Landau theory* of superconductivity. Superconductivity arises if electrons in a crystal are attracted by the effects of the elastic forces so strongly that the attraction overcomes the Coulomb repulsion. Then they form Cooper pairs which can form a condensate very similar to the bosonic helium atoms. In the absence of electric fields, the mean-field approximation to the effective action is

$$\frac{1}{T}\Gamma[\Phi]=-\int d^3x\left[\frac{1}{2}\mathbf{H}^2+\frac{1}{2}(\mathbf{D}\Phi)^*\mathbf{D}\Phi+\frac{m^2}{2}|\Phi|^2+\frac{g}{4}|\Phi|^4\right]. \tag{16.62}$$

where Since the charge carriers are electron pairs, the charge of the field is twice the electronic charge, and the covariant derivative (16.7) becomes

$$\mathbf{D} = \boldsymbol{\nabla} - iq\mathbf{A}\boldsymbol{\nabla} - i\frac{2e}{\hbar c}\mathbf{A}. \tag{16.63}$$

The first line is in natural units with $\hbar = c = 1$, the second line in physical cgs units. The magnetic field is the curl of the vector potential:

$$\mathbf{H}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{x}). \tag{16.64}$$

The time-independent equations of motion are

$$\left(-i\boldsymbol{\nabla} - q\mathbf{A}\right)^2 \Phi + m^2\Phi + g|\Phi|^2\Phi = 0 \tag{16.65}$$

$$\boldsymbol{\nabla} \times \mathbf{H} = \mathbf{j} \tag{16.66}$$

where $\mathbf{j}$ is defined as the current operator of the matter field

$$\mathbf{j} = \frac{q}{2i}\Phi^* \overset{\leftrightarrow}{\boldsymbol{\nabla}} \Phi - q^2|\Phi|^2\mathbf{A}. \tag{16.67}$$

In order to establish contact with the case of a superconductor, we again insert a temperature dependent mass term

$$m^2 = \mu^2\left(\frac{T}{T_c} - 1\right) = -\mu^2\tau \tag{16.68}$$

thereby choosing the minus sign since our interest will be focussed on the regime below T_c.

16.4 Two Natural Length Scales

Before proceeding it is useful to introduce reduced field quantities and define

$$\psi = \frac{\Phi}{|\Phi_0|} \tag{16.69}$$

with

$$|\Phi^0| = \sqrt{-\frac{\mu^2}{g}} = \frac{\mu}{\sqrt{g}}\sqrt{\tau} \tag{16.70}$$

being the nonzero vacuum expectation of the φ-field for $T < T_c0$. Also we define a length scale associated with the mass of the Φ-particle

$$\xi(\tau) = \frac{1}{\mu\sqrt{2}}, \tag{16.71}$$

and with that of the photon, after eating up the Nambu-Goldstone boson

$$\lambda(\tau) = \frac{1}{q|\Phi_0|} = \frac{\sqrt{g}}{q\mu\sqrt{\tau}} = \frac{\sqrt{g}}{q}\xi(\tau). \tag{16.72}$$

The first length scale is usually referred to as coherence length, the second as penetration depth for reasons which will become plausible soon. The ratio of the two length scales is an important temperature independent material constant denoted by κ:

$$\kappa \equiv \frac{\lambda(\tau)}{\xi(\tau)} = \frac{\sqrt{g}}{q}, \tag{16.73}$$

which measures the ratio between the coupling strength g with respect to q^2.

The coherence length is used to introduce a reduced dimensional vector potential

$$\mathbf{a} = q\xi(\tau)\mathbf{A} \tag{16.74}$$

and a reduced magnetic field

$$\mathbf{h} = \kappa\boldsymbol{\nabla}\times\mathbf{a} = q\kappa\lambda(\tau)\boldsymbol{\nabla}\times\mathbf{A}. \tag{16.75}$$

In the absence of a magnetic field, the action may then be expressed as

$$\frac{1}{T}\Gamma\left[\Phi\right] = -4f_c\xi^3\bar{F}. \tag{16.76}$$

where f_c is the so-called condensation energy density:

$$f_c = \frac{\Phi_0^2 m^2}{4} = -\frac{m^4}{4g} = -\frac{\mu^4}{4g}\tau, \tag{16.77}$$

and $\bar{F}$ is the reduced free energy

$$\bar{F} = \frac{1}{\xi^3}\int d^3x\left[\frac{1}{2}\left|\xi(\tau)(\boldsymbol{\nabla}-i\mathbf{a})\psi\right|^2 - \frac{1}{2}|\psi|^2 + \frac{1}{4}|\psi|^4 + \frac{1}{2}\lambda^2(\tau)\mathbf{h}^2\right]. \tag{16.78}$$

Note that h measures the magnetic field in units of

$$H_0 = \sqrt{2}H_c \equiv \frac{1}{q\lambda\xi} = \sqrt{m^2\Phi_0^2} = 2\sqrt{f_c} \tag{16.79}$$

where H_c is the value at which the magnetic energy density $H_c^2/2$ equals the condensation energy density f_c.

If we agree to measure all lengths x in multiples of the coherence length ξ, $\bar{F}$ becomes simply

$$\bar{F} = \int d^3x\left[\frac{1}{2}\left|(\boldsymbol{\nabla}-i\mathbf{a})\,\psi\right|^2 - \frac{1}{2}|\psi|^2 + \frac{1}{4}|\psi|^4 + \mathbf{h}^2\right]. \tag{16.80}$$

In the reduced variables the equations of motion are simply

$$(i\nabla + \mathbf{a})^2 \psi = \psi - |\psi|^2\psi, \tag{16.81}$$

$$\kappa\nabla \times \mathbf{h} = \kappa^2\nabla \times (\nabla \times \mathbf{a}) = \kappa^2[\nabla^2\mathbf{a} - \nabla(\nabla \cdot \mathbf{a})] = \mathbf{j}, \tag{16.82}$$

where $\mathbf{j}$ is the current (16.67) in natural units

$$\mathbf{j} = \frac{1}{2i}\psi^* \overleftrightarrow{\nabla} \psi - |\psi|^2\mathbf{a}. \tag{16.83}$$

Let us also write down these equations in the polar field parametrization

$$\psi(x) = \rho(x)e^{i\gamma(x)}. \tag{16.84}$$

It is convenient to absorb the gradient of $\gamma(\mathbf{x})$ into the vector potential, and go over to the field

$$\mathbf{a} \to \mathbf{a} - \nabla\gamma, \tag{16.85}$$

This brings $\bar{F}$ to the simple form

$$\bar{F} = \int dx \left\{\frac{1}{2}|(\nabla - i\mathbf{a})\rho|^2 - \frac{1}{2}\rho^2 + \frac{1}{4}\rho^4 + (\nabla \times \mathbf{a})^2\right\}, \tag{16.86}$$

and the field equations (16.81) and (16.82) becoeme

$$\left(-\nabla^2 + \mathbf{a}^2 - 1 + \rho^2\right)^2 \rho = 0, \tag{16.87}$$

$$\kappa\nabla \times \mathbf{h} = \kappa^2\nabla \times (\nabla \times \mathbf{a}) = \kappa^2[\nabla^2\mathbf{a} - \nabla(\nabla \cdot \mathbf{a})] = -\rho^2\mathbf{a}. \tag{16.88}$$

These will be most suitable for a upcoming discus sions.

16.5 Planar Domain Wall

As it was mentioned earlier, it has been known for a long time that superconductors have the tendency of expelling magnetic fields (Meissner effect). Let us study what the free energy (16.86) has to say about this magnetic phenomenon. In order to gain some rough ideas it is useful to consider a sample with a magnetic field pointing in x direction. Let us allow for variations of the system only along the z-coordinate. We may choose the vector potential $\mathbf{a}_0$ to point purely into the x-direction. If we denote the x-component of $a(z) \equiv a_0(z)$, the fields are

$$h_y(z) = \kappa a'(z), \quad h_x = h_y = 0. \tag{16.89}$$

The reduced free energy density reads

$$\bar{f} = \frac{1}{2}\rho'^2 - \frac{1}{2}\rho^2 + \frac{1}{4}\rho^4 + a^2\rho^2 + \kappa^2 a'^2, \tag{16.90}$$

whose extremization yields the equations of motion

$$-\rho'' + a^2\rho = \rho - \rho^3 \tag{16.91}$$

$$\kappa^2 a'' = a\rho^2. \tag{16.92}$$

Differentiating (16.92) and inserting (16.89), we obtain

$$\kappa^2\rho^2\frac{d}{dz}\left(\frac{1}{\rho^2}\frac{dh}{dz}\right) = \kappa^2\left(h'' - \frac{2h'\rho'}{\rho}\right) = h\rho^2. \tag{16.93}$$

Inserting (16.92) into (16.91) yields

$$-\rho'' + \kappa^2\frac{h'^2}{\rho^3} = \rho - \rho^3. \tag{16.94}$$

The last two equations can be used as coupled differential equations for h and ρ.

If these two field are known, the vector potential may be calculated from (16.92) as

$$a = \frac{a''}{\rho^2} = \frac{h'}{\rho^2}. \tag{16.95}$$

This equation gives an immediate result: A constant magnetic field can exist only for $\rho = 0$, i.e., if the system has no spontaneous symmetry breakdown. If we assume, conversely, that $\rho = \text{const} \neq 0$, then Eq. (16.91) shows that also a^2 is a constant, $a^2 = \left(1-\rho^2\right)/\rho$, implying once more from Eq. from (16.95) that h' is a constant. The contradiction is resolved only for $\rho = 1$, in which case (16.91) gives $a = 0$, and (16.95) enforces $h' = 0$. Then Eq. (16.93) shows that only $h = 0$ is a consistent solution. Therefore, constant solutions have only the two alternatives

$$h = \text{const} \neq 0, \quad \rho = 0, \quad \textit{normal phase} \tag{16.96}$$

$$h = 0, \quad \rho = 1, \quad \textit{superconductive phase.} \tag{16.97}$$

The second alternative exhibits the experimentally observed Meissner effect that the superconductive state does not permit the presence of a magnetic field.

Consider now z-dependent field configurations. In order to simplify the discussion let us first look at two limiting situations:

Case I: $\kappa \ll 1/\sqrt{2}$

This corresponds to a very short penetration depth of the magnetic field which may propagate only over length scales $\lambda(T) = \kappa\xi(\tau)$ or, in natural units, $z \sim 1$, i.e., it has a unit range. For very small κ, Eq. (16.94) becomes

$$\rho'' \approx \rho\left(1-\rho^2\right), \tag{16.98}$$

which can be integrated by multiplying it with ρ' to find

$$-\rho'^2 \approx \frac{1}{2}\left(1-\rho^2\right)^2 + E. \tag{16.99}$$

If the system is in the superconductive state for large z, the field satisfy the boundary condition corresponding to the alternative (16.96), such that $\rho \to 1$ for $z \to \infty$. Inserting this into (16.99) we see that the constant of integration E must be zero. Integrating the resulting equation further gives

$$z = \sqrt{2}\int \frac{d\rho}{1-\rho^2} = \sqrt{2}\,\text{atanh}\,\rho, \tag{16.100}$$

or

$$\rho(z) = \tanh\frac{z}{\sqrt{2}}. \tag{16.101}$$

The field configuration is displayed as the right-hand branch in the upper part of Fig. 16.1.

For $z<0$, the solution (16.101) becomes meaningless, since $\rho>0$ by definition. We can continue the solution into this regime by matching it with the lower of the trivial solution (16.97):

$$h = \text{const}, \quad \rho = 0, \tag{16.102}$$

which is shown as the left-hand branch in the upper part of Fig. 16.1.

The size of the constant magnetic field in the first case is determined by the fact that the free energy density must be the same at large positive and negative z. Otherwise, there would be energy flow. Inserting (16.99) for $E=0$ into (16.90), it becomes approximately

$$\hat{f} \approx -\frac{1}{4} + \frac{1}{2}a^2\rho^2 + \frac{1}{2}h^2. \tag{16.103}$$

For large z where $h=a=0$ and $\rho=1$, this is equal to $-1/4$. For large negative z, $\bar{f}$ is equal to h^2. Hence the constant h in the normal phase is equal to

$$h = h_c = \frac{1}{\sqrt{2}} \tag{16.104}$$

Within the region around $z \approx 0, h$ drops to zero over a unit length scale determined by (16.92) which is very short compared with the length $1/\kappa$ over which ρ varies (this is precisely the coherence length). If we plot the transition region against z, the field h jumps abruptly to zero from $h=h_c$ while ρ has a smooth increase. The full approximate solution plotted in Fig. 16.1 is

$$h(z) \approx h_c\Theta(-z), \tag{16.105}$$
$$\rho(z) \approx \tanh\frac{z}{\sqrt{2}}. \tag{16.106}$$

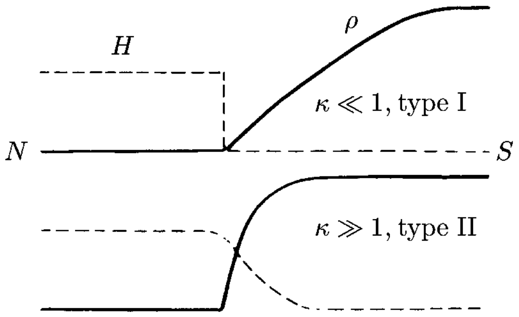


FIGURE 16.1 Dependence of order parameter ρ and magnetic field H on the reduced distance z for a planar domain wall between the normal and superconductive phases. The magnetic field points parallel to the wall.

Case II: $\kappa \gg 1/\sqrt{2}$

Consider now the opposite limit of a very large penetration depth. Here we approximate (16.94) by

$$\kappa^2 h'^2 \approx \rho^4 \left(1-\rho^2\right). \qquad (16.107)$$

implying that we may omit the gradient term ρ'' in Eq. (16.91):

$$a^2 \rho \approx \rho \left(1-\rho^2\right). \qquad (16.108)$$

Let us calculate ρ again by starting out with $\rho = 1$ at $z = \infty$. Then h must decrease for positive z and we have to take the positive square root

$$\kappa h' = \rho^2 \sqrt{1-\rho^2}. \qquad (16.109)$$

From Eq. (16.93), one the other hand, we obtain

$$h \approx \kappa^2 \frac{d}{dz}\left(\frac{1}{\rho^2}\frac{d}{dz}h\right) = -\kappa \frac{d}{dz}\sqrt{1-\rho^2}. \qquad (16.110)$$

It is convenient to introduce the abbreviation

$$u \equiv \sqrt{1-\rho^2}, \qquad (16.111)$$

such that (16.110) becomes

$$h = -\kappa u', \qquad (16.112)$$

and (16.109) turns into the simple differential equation

$$\kappa^2 u'' = \left(1-u^2\right) u. \qquad (16.113)$$

After multiplying this with u', and integrating, we find

$$\kappa^2 u'^2 = u^2\left(1-\frac{u^2}{2}\right)+\text{const.} \tag{16.114}$$

Inposing the asymptotic condition that at large z the order field ρ goes against 1, the function $u(z)$ must vanish in this limit, fixing the constant to zero. The equation is then solved by

$$z-z_0=\kappa\int\frac{du}{u}\frac{1}{\sqrt{1-u^2/2}}=\kappa\text{atanh}\frac{1}{\sqrt{1-u^2/2}} \tag{16.115}$$

or

$$u(z)=\frac{\sqrt{2}}{\cosh[(z-z_0)/\kappa]}. \tag{16.116}$$

From (16.111) we find

$$\rho=\sqrt{1-\frac{2}{\cosh^2[(z-z_0)/\kappa]}}. \tag{16.117}$$

As z comes in from large positive values, ρ decreases. We can arrange it to become zero at $z=0$ if we choose z_0 such that

$$\sinh(z_0/\kappa)=1. \tag{16.118}$$

The magnetic field is then from Eq. (16.112):

$$h(z)=\frac{\sqrt{2}\sinh[(z-z_0)/\kappa]}{\cosh^2[(z-z_0)/\kappa]}. \tag{16.119}$$

It is zero at $z=\infty$, and and becomes gradually stronger as approaches $z=0$, where it reaches the value

$$h=h_c=\frac{1}{\sqrt{2}} \tag{16.120}$$

as before. From there on we may again match the trivial solution continuously by setting

$$h\equiv h_c,\quad \rho\equiv 0;\quad z<0. \tag{16.121}$$

The full solution shown in Fig. 16.1 is then

$$\rho(z) = \Theta(z)\sqrt{1-\frac{2}{\cosh^2[(z-z_0)/\kappa]}}, \tag{16.122}$$

$$h(z) = \Theta(-z)h_c+\Theta(z)\frac{\sqrt{2}\sinh[(z-z_0)/\kappa]}{\cosh^2[(z-z_0)/\kappa]}. \tag{16.123}$$

The ranges over which h and ρ vary are of equal order κ, or in physical units of order $\lambda = \kappa\xi$.

Case III: $\kappa = 1/\sqrt{2}$

Here a trial ansatz

$$h = \frac{1}{\sqrt{2}}\left(1-\rho^2\right) \tag{16.124}$$

can be inserted into (16.93), with the result

$$\left(1-\rho^2\right)\rho^2 = -\rho\rho'' + \rho'^2. \tag{16.125}$$

This, in turn, happens to coincide with the other equation (16.94), thus verifying the ansatz (16.124). For $z = \infty$ The fields start out with $\rho = 1$ and $h = 0$, and go to $\rho = 0$ and $h = h_c = 1/\sqrt{2}$ for $z = -\infty$.

Equation (16.125) takes a particularly appealing form if we consider the auxiliary function $\sigma(z)$ defined by $\rho(z) \equiv e^{\sigma(z)/2}$. Then

$$\rho' = \frac{1}{2}\sigma' e^{\sigma/2}, \qquad \rho'' = \frac{1}{2}\sigma'' e^{\sigma/2} + \frac{1}{k}\sigma'^2 e^{\sigma/2} \tag{16.126}$$

and we may rewrite (16.125) as

$$-\left(1-e^\sigma\right) = \frac{\rho''}{\rho} - \frac{\rho'^2}{\rho^2} = \frac{1}{2}\sigma''. \tag{16.127}$$

This can be integrated to

$$e^\sigma - 1 - \sigma = \frac{\sigma'^2}{4}, \tag{16.128}$$

which is integrated to

$$z = -\frac{1}{2}\int_a^\sigma \frac{d\sigma'}{\sqrt{e^{\sigma'} - 1 - \sigma'}}. \tag{16.129}$$

For $z \longrightarrow \infty$, the solution h $\sigma(z)$ goes to zero like $e^{-z/\sqrt{2}}$, such that $\rho \longrightarrow 1$. For $z \longrightarrow -\infty$, it becomes more an more negative like $\sigma(z) \sim -z^2/4$, such that $\rho(z) \longrightarrow 0$ exponentiall fast.

For intermediate values κ, the solutions have to be found numerically. They all look qualitatively similar. The ratio κ of penetration depth to coherence length determines how far the magnetic field invades into the superconductive region relative to the coherence length.

16.6 Surface Energy

Consider the energy per unit length for these classical fields as they follow from Eq. (16.90). Inserting the equations of motion and performing one partial integration renders the much simpler expression for the energy per area $\bar{A}$, bith in natural units:

$$\frac{\bar{F}}{\bar{A}} = \int dz f = \int dz \left(-\frac{1}{4}\rho^4 + \frac{1}{2}h^2 \right). \tag{16.130}$$

Obviously, the classical solution with an absolute minimum is $h = 0, \rho = 1$. In order to enforce the previously discussed configurations, an external magnetic field is needed, and we must minimize the reduced *magnetic enthalpy* per unit length area

$$\frac{\bar{G}}{\bar{A}} = \int dz \left[-\frac{1}{4}\rho^4 + \frac{1}{2}h^2 - h\, h_{\rm ext} \right], \tag{16.131}$$

where we have subtracted a term

$$m\, h_{\rm ext} = h\, h_{\rm ext}, \tag{16.132}$$

in which the reduced magnetization $m \equiv \partial_h \bar{G}/\bar{A} = h$ is coupled to the reduced external magnetic field. Such a term does change the differential equations (16.91) and (16.92) for a and ρ, since it is a pure surface term $h_{\rm ext}\partial_z a$.

For $z \longrightarrow -\infty$, where $\rho \longrightarrow 0$ and $h \longrightarrow h_c$, the enthalpy goes asymptotically against

$$\frac{\bar{G}}{\bar{A}} \approx \int dz \left[\frac{1}{2}h_c^2 - h_c\, h_{\rm ext} \right]. \tag{16.133}$$

For $z \longrightarrow \infty$, on the other hand, where the size of the order field order field goes to 1 and $h \longrightarrow 0$, the asymptotic value is

$$\frac{\bar{G}}{\bar{A}} \approx \int dz \left(-\frac{1}{4} \right). \tag{16.134}$$

Thus both asymptotic regimes have the same magnetic enthalpy for the particular external field $h_{\rm ext} = h_c = 1/\sqrt{2}$. If the energy was smaller in one regime, the wall between superconductive and normal phase would start moving towards one side such as to decrease the energy. This would go on until the system is uniform. Thus we conclude: For $h > h_c$, the system is uniformly normal, for $h < h_c$ uniformly super-conductive.

We now calculate the energy stored in the finite region around $z = 0$ at the critical magnetic field $h_{\rm ext} = h_c$. There the density deviates only slightly from the asymptotic form, and we must evaluate the expression

$$\frac{\bar{G} - \bar{G}_{as}}{\bar{A}} = \int_{-\infty}^{\infty} dz \left(-\frac{1}{4}\rho^4 + \frac{1}{2}h^2 - \frac{1}{\sqrt{2}}h + \frac{1}{4} \right). \tag{16.135}$$

Note the special properties of the case $\kappa = 1/\sqrt{2}$: Inserting (16.124), the surface energy is seen to vanishes.

When inserting into (16.135) the $\kappa \gg 1$ -solutions (16.122) and (16.123), we find, using Eqs. (16.111) and (16.112)), the negative energy

$$\begin{aligned}\frac{\bar{G}-\bar{G}_{as}}{\bar{A}} &= \int_{-\infty}^{\infty} dz \left[u^2\left(1-\frac{u^2}{2}\right)-\frac{1}{\sqrt{2}}u\left(1-\frac{u^2}{2}\right)^{1/2}\right] \\ &= \int_{-\infty}^{\infty} dz \left[u\sqrt{1-\frac{u^2}{2}}-\frac{1}{\sqrt{2}}\right]\frac{du}{dz} = \left(-\frac{2}{3}\sqrt{2}-\frac{1}{2}\right) < 0. \qquad (16.136)\end{aligned}$$

The same sign holds for all $\kappa > 1/\sqrt{2}$.

For $\kappa \ll 1$, on the other hand, the enthalpy (16.135) vanishes in the superconducting phase for $z > 0$, where $\rho = 1$ and $h = 0$. In the normal phase, where $h = h_c$ by Eq. (16.104), we find

$$\frac{\bar{G}-\bar{G}_{as}}{\bar{A}} = \int_{-\infty}^{0} dz \frac{1}{4}\left(1-\rho^4\right) = \frac{1}{2\sqrt{2}}\int_0^1 d\rho\,(1+\rho^2), \qquad (16.137)$$

which is positive for all $\kappa < 1/\sqrt{2}$.

Thus we conclude: In superconductors with $\kappa > 1/\sqrt{2}$, it is energetically more favorable to form a wall in which the magnetic field develops from zero up to h_c than to have a uniform field configuration. For $\kappa < 1/\sqrt{2}$, the opposite is true. The first case is referred to as a soft or type-II superconductor, the second as a hard type-I superconductor.

16.7 Single Vortex Line and Critical Field H_{c1}

Consider now a type-II superconductor in small external magnetic field $H_{\rm ext}$, where it is in the state of broken symmetry with a uniform order field $\Phi = \Phi_0$. When increasing $H_{\rm ext}$, there will be a critical value H_{c1} where the field lines first begin to invade the superconductor. We expect this to happen in the form of a quantized magnetic *flux tubes*. which are *vortex lines* of supercurrent. When increasing $H_{\rm ext}$ further, more and more flux tubes will perforate the superconductor, until the critical magnetic field H_c is reached, where the sample becomes normally conducting. The regime between H_{c1} and H_c is called the *mixed state* of the type-II superconductor.

The quantum of flux carried by each flux tube is

$$\Phi_0 = \frac{ch}{2e} \approx 2 \times 10^{-7} \text{ gauss cm}^2 . \qquad (16.138)$$

Such a flux tube may be considered as a line-like defect in the uniform superconductor. It forms a *vortex line* of supercurrent, very similar to the vortex lines in superfluid helium discussed in Section 15.4. The two objects possess, however, quite different physical properties, as we shall see.

Suppose the system is in the superconductive state without an external voltage so that there is no net current $\mathbf{j}$. Suppose a flux tube runs along the z-axis. Then we can use the current (16.83) to find the vector potential

$$\mathbf{a} = -\frac{\mathbf{j}}{|\psi|^2} + \frac{1}{2i}\frac{1}{|\psi|^2}\psi^\dagger \overset{\leftrightarrow}{\boldsymbol{\nabla}} \psi. \tag{16.139}$$

Far away from the fluc tube, the state is undisturbed, the current $\mathbf{j}$ vanishes, and we have the relation

$$\mathbf{a} = \frac{1}{2i}\frac{1}{|\psi|^2}\psi^\dagger \overset{\leftrightarrow}{\boldsymbol{\nabla}} \psi. \tag{16.140}$$

In polar decomposition of the field $\psi(\mathbf{x}) = \rho(\mathbf{x})e^{i\gamma(\mathbf{x})}$, the derivative of $\rho(\mathbf{x})$ cancels, and $\mathbf{a}(\mathbf{x})$ becomes the gradient of the phase of the order parameter:

$$\mathbf{a}(\mathbf{x}) = \boldsymbol{\nabla}_i\gamma(\mathbf{x}). \tag{16.141}$$

Here we can establish contact withthe discussion of superfluid helim in Section 15.4. There the superflow velocity was proportional to the gradient of a phase angle variable $\gamma(\mathbf{x})$. The periodicity of $\gamma(\mathbf{x})$ led to the quantization rule that, when taking the integral over $d\gamma(\mathbf{x})$ along a closed circuit around the vortex line, it had to be an integral multiple of 2π [recall Eq. (15.103)]. The same rule applies here:

$$\oint_B d\gamma(\mathbf{x}) = \oint_B d\mathbf{x}\cdot\boldsymbol{\nabla}\gamma(\mathbf{x}) = 2\pi n. \tag{16.142}$$

By Stokes' theorem, this is equal to the integral $\int d\mathbf{S}\cdot\boldsymbol{\nabla}\times\mathbf{a}$, where $d\mathbf{S}$ is a surface element of the area enclosed by the circuit. Since $\mathbf{h} = \kappa(\boldsymbol{\nabla}\times\mathbf{a})$is the magnetic field in natural units [recall (16.85)], the integral (16.142) is directly proportional to the magnetic flux through the area of the circuit

$$\bar{\boldsymbol{\Phi}} = \int_{S_B} d\mathbf{S}\cdot\mathbf{h} = \kappa\int d\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{a}) = \kappa\oint_B d\mathbf{x}\cdot\mathbf{a} = \kappa\oint_B d\mathbf{x}\cdot\boldsymbol{\nabla}\gamma = 2\pi n\kappa. \tag{16.143}$$

This holds in natural units, indicated by a bar on top of $\boldsymbol{\Phi}$, in which $\hbar = c = 1$, the vector potential is given by (16.74), and $\mathbf{x}$ is measure in units of the coherence length.

The quantization condition in physical cgs units follows from the same argument applied to the original current (16.67). Remembering

$$q = \frac{2e}{\hbar c}. \tag{16.144}$$

from (16.63), the relation (16.140) reads

$$\mathbf{A} = \frac{2e}{2i\hbar c}\frac{1}{|\psi|^2}\psi^\dagger \overset{\leftrightarrow}{\boldsymbol{\nabla}} \psi, \tag{16.145}$$

and (16.141) becomes

$$\mathbf{A}(\mathbf{x}) = \frac{\hbar c}{2e}\boldsymbol{\nabla}_i\gamma(\mathbf{x}) = \frac{\boldsymbol{\Phi}_0}{2\pi}\boldsymbol{\nabla}_i\gamma(\mathbf{x}). \tag{16.146}$$

The magnetic flux integral in cgs units is therefore

$$\boldsymbol{\Phi} = \int_{S_B} d\mathbf{S}\cdot\mathbf{H} = \int d\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{A}) = \oint_B d\mathbf{x}\cdot\mathbf{A} = \frac{\Phi_0}{2\pi}\oint_B d\mathbf{x}\cdot\boldsymbol{\nabla}\gamma = n\boldsymbol{\Phi}_0. \tag{16.147}$$

It is an integer multiple of the fundamental flux (16.138).

It is instructive to performing the circuit integral (16.143) once more around a circle close to the flux tube, where the current in Eq. (16.139) no longer vanishes. The angular integral $\oint d\mathbf{x}\cdot\boldsymbol{\nabla}\gamma$ still has to be equal to $2\pi n$, and we find the quantization rule

$$\oint_B d\mathbf{x}\cdot\left(\mathbf{A} + \frac{\mathbf{j}}{|\psi|^2}\right) = 2\pi n, \tag{16.148}$$

or

$$\bar{\boldsymbol{\Phi}} + \frac{1}{|\psi|^2}\oint_B d\mathbf{x}\cdot\mathbf{j} = 2\pi n\kappa, \tag{16.149}$$

This shows that through the smaller circuit, which enloses fewer magnetic field lines, there is an increasing contribution of the supercurrent around the center of the vortex line, which keeps the sum of the two contributions in (16.149) equal to $2\pi n\kappa$. This shows that the flux tube is indeed a vortex line with respect to supercurrent. The circular current density must be inversely proportional to the distance. This behavior will be derived explicitly in Eq. (16.191).

Quantitatively, we can find the properties of a vortex line by solving the field equations (16.87) and (16.88) in cylindrical coordinates. Inserting the second into the first equation, we find

$$-\frac{1}{r}\frac{d}{dr}r\frac{d\rho}{dr} + \frac{\kappa^2}{\rho^3}\left(\frac{dh}{dr}\right)^2 - (1-\rho^2)\rho = 0, \tag{16.150}$$

where h denotes the z-component of $\mathbf{h}$. Forming the curl of the second equation gives the cylindrical analogue of (16.95), i.e.,

$$h = \kappa^2\frac{1}{r}\frac{d}{dr}\frac{r}{\rho^2}\frac{d}{dr}h. \tag{16.151}$$

For $r \to \infty$, we have the boundary condition $\rho = 1,\ h = 0$ (superconductive state with Meissner effect) and $\mathbf{j} = 0$ (no current). Since $\mathbf{j}$ is proportional to $\boldsymbol{\nabla}\times\mathbf{h}$ by Eq. (16.82), the last condition implies that

$$h'(r) = 0, \quad r \to \infty. \tag{16.152}$$

In cylindrical coordinates, the flux quantization condition (16.143) can be written in the form

$$\bar{\mathbf{\Phi}} = 2\pi \int_0^\infty dr\, r\, h(r) = 2\pi n\kappa. \tag{16.153}$$

Inserting here Eq. (16.151) yields

$$\bar{\mathbf{\Phi}} = 2\pi\kappa^2 \left[\frac{r}{\rho^2} h'(r)\right]_0^\infty = -2\pi\kappa^2 \left[\frac{r}{\pi^2} h'(r)\right]_{r=0}, \tag{16.154}$$

so that the quantization condition turns into a boundary condition at the origin:

$$h' \longrightarrow -\rho^2 \frac{n}{\kappa}\frac{1}{r}, \qquad \text{for} \quad r \to 0. \tag{16.155}$$

Inserting this condition into (16.150) we see that close to the origin, $\rho(r)$ satisfies the equation

$$-\frac{1}{r}\frac{d}{dr} r \frac{d}{dr}\rho(r) + \frac{n^2}{r^2}\rho - (1-\rho^2)\rho \approx 0, \tag{16.156}$$

implying the small-r behavior of $\rho(r)$:

$$\rho(r) = c_n \left(\frac{r}{\kappa}\right)^n + \mathcal{O}\left(r^{n+1}\right). \tag{16.157}$$

Reinserting this back into (16.155) we have

$$h(r) = h(0) - \frac{c_n^2}{2\kappa}\left(\frac{r}{\kappa}\right)^{2n}. \tag{16.158}$$

For large r, where $\rho \longrightarrow 1$, the differential equation (16.151) is solved by the modified Bessel function K_0, with some proportionality factor α:

$$h(r) \longrightarrow \alpha K_0\left(\frac{r}{\kappa}\right), \quad r \longrightarrow \infty. \tag{16.159}$$

More explicitly, the limit is

$$h(r) \longrightarrow \alpha\sqrt{\pi\kappa/2r}\,e^{-r/\kappa}., \quad r \longrightarrow \infty. \tag{16.160}$$

Consider now the deep type-II regime where $\kappa \gg 1/\sqrt{2}$. There $\rho(r)$ goes rapidly to unity, as compared to the length scale over which $h(r)$ changes, which is κ in the present natural units. Therefore, the behavior (16.159) holds very close to the origin. We can determine α by matching (16.159) to (16.155) and find (since $K_0'(r) = -K_1(r) \approx -l/r$ for small r)

$$\alpha = \frac{n}{\kappa} \tag{16.161}$$

In general, $h(r)$ and $\rho(r)$ have to be found numerically. A typical solution for $n=1$ is shown in Fig. 16.2 for $\kappa = 10$.

The energy of a vortex line can be calculated hy using (16.86). Inserting the equations of motion (16.87) and (16.88), and subtracting the condensation energy, we obtain from (16.130)]

$$\Delta\bar{F}_{\rm vort} = \bar{F}_{\rm vort} - \bar{F}_c = \frac{1}{2}\int d^3x \left[\frac{1}{2}(1-\rho^4) + h^2\right]. \qquad (16.162)$$

For $\kappa \gg 1/\sqrt{2}$, we may neglect the small radius $r \leq 1$, over which ρ increases quickly from zero to its asymptotic value $\rho = 1$. Above $r \approx 1$ the magnetic field for r $r \leq \kappa$ is given by (16.159). Inserting this into (16.150) with (16.157), we find and for $r \leq \kappa$, h is given by (16.159). Inserting this into (16.150) with (16.157), we find

$$\rho(r) \approx 1 - \frac{n^2}{2r^2}. \qquad (16.163)$$

Thus the region $1 \leq r \leq \kappa$ yields an energy per unit length

$$\frac{1}{L}\bar{F}_{\rm vort} = \frac{1}{2}2\pi\int_1^\kappa drr\left[\frac{1}{2}(1-\rho^4)+h^2\right] = \pi n^2\int_1^\kappa drr\left[\frac{1}{r^2}+\frac{1}{\kappa^2}K_0^2\left(\frac{r}{\kappa}\right)\right]. \qquad (16.164)$$

For $\kappa \to \infty$, the second integral becomes a constant, since $\int_0^\infty dx\, x\, K_0^2(x) = 1/2$. The first integral, on th other hand, has a logarithmic divergence so that we find

$$\frac{1}{L}\bar{F}_{\rm vort} \approx \pi n^2[\log\kappa + \quad \text{const.}]. \qquad (16.165)$$

A more careful evaluation if the integral yields $\pi n^2(\log\kappa + 0.08)$.

Let us now see at which external magnetic field such a vortex line can form. For this we consider again the magnetic enthalpy (16.131), and subtract from $\bar{G}_{\rm vort}/L$, the magnetic $\bar{G}_{\rm vort}/L$ coupling hh^{ext} so that, per unit length

$$\frac{1}{L}\bar{G}_h = \pi n^2(\log\kappa + 0.08) - 2\pi\int_0^\infty dr\, r\, h\, h^{ext}. \qquad (16.166)$$

But the integral over h is simply the flux quantum (16.143) associated with the vortex line, such that

$$\frac{1}{L}\bar{G}_h = \pi n^2(\log\kappa + 0.08) - 2\pi n\kappa\, h^{ext}. \qquad (16.167)$$

When this is smaller than zero, a vortex line will invade the superconductor along the z-axis. The associated critical magnetic field is

$$h_{c1} = \frac{n}{2}\frac{\log\kappa + 0.08}{\kappa}. \qquad (16.168)$$

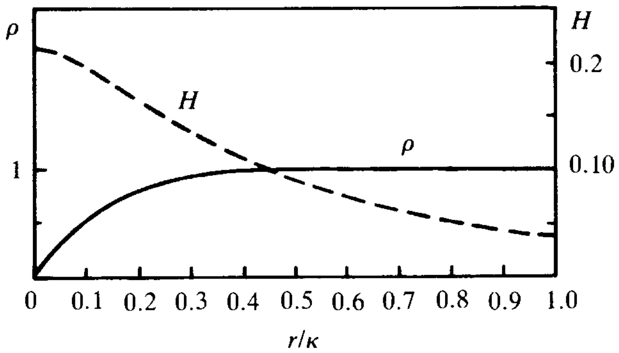


FIGURE 16.2 Order parameter ρ, and the magnetic field h for an $n = 1$ vortex line in a deep type-II superconductor with $K = 10$.

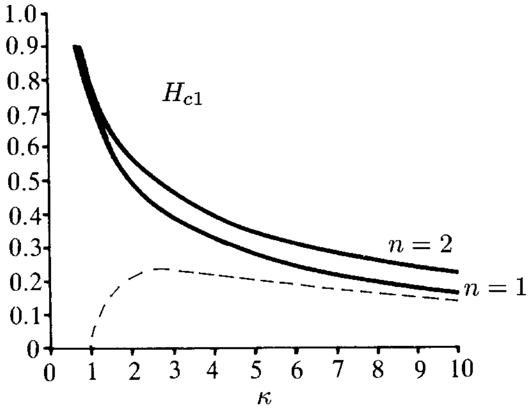


FIGURE 16.3 Critical field h_{c1} at which a vortex line of strength n forms when it first invades a type-II superconductor, as a function of the parameter κ. The dotted line indicates the asymptotic result $(1/2\kappa)\log\kappa$ of Eq. (16.168). The magnetic field h_c is measured in units of $\sqrt{2}H_c$ where H_c is the magnetic field at which the magnetic energy equals the condensation energy.

TABLE 16.1 The different critical magnetic fields in units of gauss for various impurities.

material	H_c	H_{c1}	H_{c2}	T_c/K
Pb	550	550	550	4.2
0.85 Pb, 0.15 Ir	650	250	3040	4.2
0.75 Pb, 0.25 In	570	200	3500	4.2
0.70 Pb, 0.30 Tl	430	145	2920	4.2
0.976 Pb, 0.024 Hg	580	340	1460	4.2
0.912 Pb , 0.088 Bi	675	245	3250	4.2
Nb	1608	1300	2680	4.2
0.5 Nb, 0.5 Ta	252	—	1370	5.6

For large κ, this field can be quite small. The asymptotic result is compared with a numerical solution of the differential equation for $n = 1, 2, 3, \ldots$ in Fig. 16.3.

For a comparison with experiment one expresses this field in terms of the critical magnetic field $h_c = 1/\sqrt{2}$ and measures the ratio

$$\frac{H_{c1}}{H_c} = \frac{n}{\sqrt{2}\kappa}(\log\kappa + 0.08). \tag{16.169}$$

If the magnetic field is increased above H_{c1}, many flux tubes will invade the type-II superconductor. These turn out to repell each other. The repulsion energy can be minimized if the flux tubes form a hexagonal array, as shown in Fig. 16.4. The tubes will perform thermal fluctuations, which may be so violent that the superflow experiences dissipation. The taming of these fluctuations is one of the main problems in high-temperature superconductors. It is usually don by introducing lattice defects at which the votex lines are pinned.

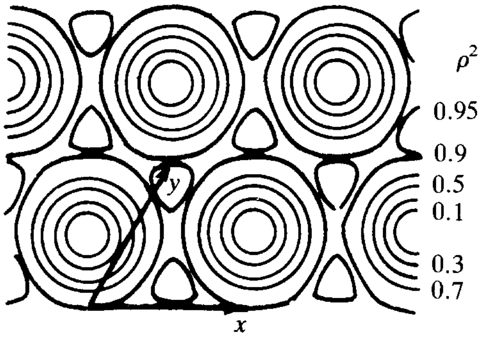


FIGURE 16.4 Spatial distribution magnetization of the order parameter $\rho(\mathbf{x})$ in a typical mixed state in which the vortex lines form a hexagonal lattice (from W.M. Kleiner et al., See References.)

16.8 Critical Field H_{c2} where Superconductivity is Destroyed

When considering planar z-dependent field configurations we found that for $H > H_c$, the order parameter vanishes and the magnetic field perforates the superconductor. Experimentally this is not true. The symmetric field inside the sample to increase markedly at a larger field value H_{c2}, which in a deep type-II superconductor can lie far above H_c. We shall now see, by allowing for a more general space dependence, that a non-zero field ρ exists up to a magnetic field

$$H_{c2} = \kappa\sqrt{2}H_c > H_c \quad \text{for} \quad \kappa > 1/\sqrt{2}. \tag{16.170}$$

Only for $H > H_{c2}$ the field $\rho(\mathbf{x}$ is forced to zero in the entire system, which then a normal conductor.

In order to calculate the size of H_{c2}, we observe that for H very close to H_{c2}, the order parameter must be very small. Hence we can linearize the field equation (16.81), writing it approximately as

$$(i\boldsymbol{\nabla} + \mathbf{a})^2 \psi \approx \psi. \tag{16.171}$$

For a uniform magnetic field in the z-direction, we may choose different forms of the vector potential $\mathbf{a}$ which differ by gauge transformations. A convenient form is

$$\mathbf{a} = \frac{h}{\kappa}(0, x, 0). \tag{16.172}$$

Then ψ satisfies the Schrödinger equation

$$\left[-\partial_x^2 + \left(i\partial_y + \frac{h}{\kappa}x\right)^2 - \partial_z^2\right]\psi = \psi. \tag{16.173}$$

This may be solved by a general ansatz

$$\psi(x, y, z) = e^{ik_z z + ik_y y}\chi(x), \tag{16.174}$$

where $\chi(x)$ satisfies the differential equation

$$\left\{-\frac{d^2}{dx^2} + \left[\left(-k_y + \frac{h}{\kappa}x\right)^2 - \left(1 - k_z^2\right)\right]\right\}\chi(x) = 0. \tag{16.175}$$

This is the Schrödinger equation of a linear oscillator of frequency $\omega = h/\kappa$, with the potential centered at

$$x_0 = \frac{\kappa k_y}{h}. \tag{16.176}$$

In fact, Eq. (16.175) can be written as

$$-\chi_{xx}(x) + \omega^2 (x - x_0)^2 \chi(x) = (1 - {k_z}^2)\chi(x). \tag{16.177}$$

This equation has a solution $\chi(x)$, which goes to zero for $x \to \infty$, if

$$\frac{1}{2}\left(1 - k_z^2\right) \equiv E_n = \omega\left(n + \frac{1}{2}\right) = \frac{h}{\kappa}\left(n + \frac{1}{2}\right). \tag{16.178}$$

The energy $E_n = \frac{1}{2}(1 - k_z^2)$ is bounded by 1 from above. Hence there cannot be solutions for arbitrarily large h. The highest h is supported by the ground state solution, where $n = 0$. But also this ceases to exist as h reaches the critical value h_{c2} given by

$$\frac{\omega}{2} = \frac{h}{2\kappa} = \frac{1}{2} \tag{16.179}$$

where

$$h_{c2} = \kappa. \tag{16.180}$$

Going back to physical magnetic fields, this amounts to

$$H_{c2} = \kappa\sqrt{2}H_c. \tag{16.181}$$

The wave functions of these solutions are strongly concentrated around $x \approx x_0$, implying that the system is normal almost everywhere, except for a sheet of thickness $\sqrt{\kappa/h}$, in units of the coherence length.

This sheet carries a supercurrent. Let us study its properties. If we insert $\psi(\mathbf{x})$ of Eq. (16.174) and $\mathbf{a}$ of Eq. (16.172) into Eq. (16.83) for the supercurrent, we find

$$\begin{aligned} \mathbf{j} &= \frac{1}{2i}\psi^* \overset{\leftrightarrow}{\nabla} \psi - |\psi|^2 \mathbf{a} = |\chi(x)|^2 \left[(0, k_y, k_z) - \frac{h}{\kappa}(0, x, 0)\right] \\ &= -|\chi(x)|^2 \left(0, \frac{h}{\kappa}(x - x_0), k_z\right). \end{aligned} \tag{16.182}$$

The supercondicting sheet is centered around $x = x_0$ parallel to the yz-plane. It carries no net charge flow along the x-axis. It consists of a double layer of current flowing in $\pm y$ directon for $x > x_0$ or $x < x_0$, respectively.

If the current along the z-axis is nonzero, the critical magnetic field is reduced to a lower value

$$h_{c2} \to \kappa\left(1 - k_z^2\right). \tag{16.183}$$

The sheet configuration is obviously degenerate with respect to the position x_0 of the sheet. Moreover, being in the regime of a linear Schrödinger equation, we can use the superposition principle to set up different spatial structures. For example, we may form an average over sheets in the rotated $(\cos\varphi\hat{x} + \sin\varphi\hat{y}, \hat{z})$-planes, and obtain cylindrical structures. These have a definite angular momentum around the z axis rather than a definite linear momentum k_y. Their wave function can be found directly from a vector potential

$$\mathbf{a} = \frac{h}{2\kappa}(-y, x, 0), \tag{16.184}$$

which reads in cylindrical coordinates

$$a_\varphi = \frac{h}{2\kappa}\rho, \quad a_r = 0, \quad a_z = 0. \tag{16.185}$$

The linearized field equation now becomes

$$\left[-\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{h^2}{\kappa^2}r^2\right] = \psi(z, r, \varphi) \tag{16.186}$$

and may be solved by a factorized ansatz

$$\psi(zr\varphi) = \chi(\sqrt{h/\kappa}r)e^{im\varphi}e^{ik_z z}. \tag{16.187}$$

The differential operator is the same as for a two-dimensional harmonic oscillator of frequency $\omega = h/\kappa$ and its wave functions are well known. They may be expressed in terms of the confluent hapergeometric functions ${}_1F_1(a;b;z)$ as

$$\chi(r') = e^{-r'/2}r'^{|m|/2}{}_1F_1(-n;|m|+1;r'), \tag{16.188}$$

The corresponding energy eigenvalues where $r' = \sqrt{h/\kappa r}$.

$$E = \omega\left(n + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2}\right) + k_z^2. \tag{16.189}$$

They have to be equated with $1/2(1-k_z^2)$ to obtain the highest possible magnetic field, which is again found to be

$$h_{c2} = \kappa(1-k_z^2), \tag{16.190}$$

as in (16.183). The current carried by this cylindrical solution is found by inserting (16.184) and (16.187) into (16.82). For $n=0$ and arbitrary $m>0$, we obtain

$$\begin{aligned}\mathbf{j} &= \chi^2\left(\sqrt{h/\kappa r}\right)\left[m\left(\frac{y}{r^2},-\frac{x}{r^2},0\right)+(0,0,k_z)-\frac{h}{2\kappa}(-y,x,0)\right]\\ &= \chi^2\left(\sqrt{h/\kappa r}\right)\left[k_z\mathbf{e}_z+\left(\frac{m}{r^2}-\frac{h}{2\kappa}\right)\mathbf{e}_\varphi\right]\end{aligned} \tag{16.191}$$

The wave function is non-zero within a narrow tube of diameter $\sqrt{\kappa/h}$ in units of the coherence length. Within this tube, a current is rotating clockwise around the z-axis, just as we deduced before from the qualitative discussion of Eq. (16.149). In addition, there may be an arbitrary linear current flowing in z-direction.

The magnetic enthalpy (16.131) of a type-II superconductor is always smaller than zero because of the negative interfacial energy. Therefore, states with a nonzero magnetic field will laways form for H below H_{c2}.

If the magnetic field is far below H_{c2}, the order field $\rho(\mathbf{x})$ will be so large that the quartic terms in the field equation (16.87) can no longer be neglected. The field configuration becomes inaccessible to simple analytic calculations.

17

Exactly Solvable O(N)-Symmetric ϕ^4-Theory for Large N

The functional integral representation of quantum field theory introduced in Chapter 10 has an important advantage over the operator formulation: it offer a similar freedom in changing variables of integration as ordinary integrals do. In physical applications it may often be more economic to describe the system not in terms of the most fundamental particles. In fact, many interesting phenomena in many-body systems are carried by products of funcdamental fields which will be called *composite fields* or *collective fields*.

17.1 Introduction of a Collective Field

As an example we consider a ϕ^4-theory, in which the field carries an extra index $a = 1, \dots, N$ allowing for an O(N)-degree of freedom. The generating functional is

$$Z[j] = \mathcal{N} \int \mathcal{D}\phi e^{i \int d^4x \left\{ \frac{1}{2}(\partial\phi_a)^2 - \frac{m_0^2}{2}\phi_a^2 - \frac{g}{4}\left(\phi_a^2\right)^2 + j_\mu \phi_a \right\}}, \tag{17.1}$$

where $\mathcal{N}$ is a normalization factor

$$\mathcal{N} = \left[\mathrm{Tr}\,\log\left(-\partial^2 - m_0^2\right)\right]^{1/2}. \tag{17.2}$$

We have slightly changed the convention of how the coupling constant appears in the action, replacing $g/4!$ by $g/4$, to save some numerical factors in the upcoming calculations.

The above theory of a fluctuating ϕ_a will now be tranformed into another one, in which only an O(N)-invariant collective field σ appears, which describes the phenomena carried by the composite ϕ_a^2. We can achieve this by means of an auxiliary functional

$$Z_{\rm aux} = \int \mathcal{D}\sigma e^{i\frac{1}{4g}\left(\sigma - g\phi_a^2\right)^2}. \tag{17.3}$$

The integral is of the pure Fresnel type and cannot depend on the field ϕ_a^2. Thus it is a constant and may be multiplied into (17.1) without changing the dynamics. Note that the field σ fluctuates quadratically around ϕ_a^2 (up to the factor g). Thus it contains all informations on this composite operator. In fact the classical equation of motion is simply

$$\sigma_{\rm cl} = g\phi_a^2, \tag{17.4}$$

i.e., at rhe classical level σ is equal to $g\phi_a^2$. The modifed functional

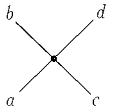
$$\begin{aligned} Z[j] &= Z_{\rm aux}\int \mathcal{D}\phi e^{i\int d^4x\left\{\frac{1}{2}(\partial\phi_a^2)^2-\frac{m_0^2}{2}\phi_a^2-\frac{g}{4}\left(\phi_a^2\right)^2+j_a\phi_a\right\}} \\ &= \int \mathcal{D}\phi\mathcal{D}\sigma e^{i\int d^4x\left\{\frac{1}{2}\phi_a\left(-\partial^2-m_0^2-\sigma\right)\phi_a+\frac{1}{4g}\sigma^2+j_a\phi_a\right\}} \end{aligned} \tag{17.5}$$

describes exactly the same theory as before.

In the presence of the collective σ-field, the ϕ_a-fields have a propagator

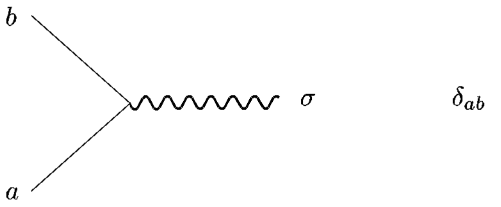
$$G_\sigma(x,x') \equiv \frac{i}{-\partial^2-m_0^2-\sigma}(x,x'). \tag{17.6}$$

Diagrammatically it is easy to understand why this is so. In the diagrams associated with the action in (17.5), the original four-vertex



$$= 3!gT_{abcd} = 2g(\delta_{ab}\delta_{cd}+\delta_{ac}\delta_{bd}+\delta_{ad}\delta_{bc}) \tag{17.7}$$

is generated by the exchange of σ. If this field is represented by a wiggly line, its interactions with the original field may be pictured by the diagram

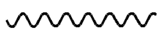


(17.8)

The quadratic part of the action in the field σ is

$$\mathcal{A}_0[\sigma] = i\frac{1}{4g}\sigma^2. \tag{17.9}$$

which corresponds to a "propagator"[1]

$G_{\sigma\sigma} =$  $= 2g.$ (17.10)

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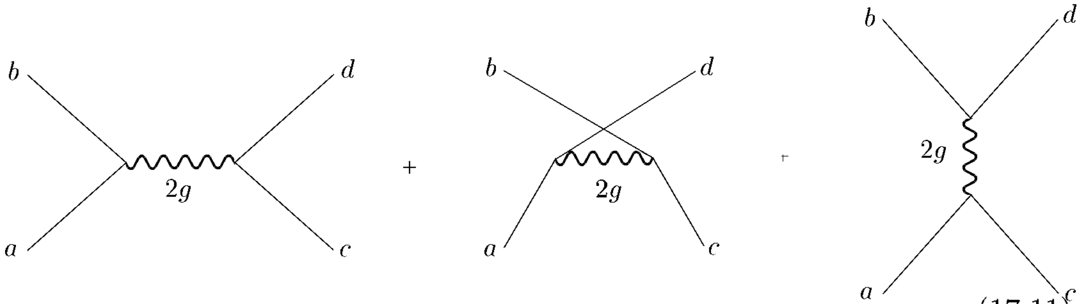
[1] The name propagator is not quite appropriate, since the σ-particle does not propagate in this lowest approximation.

The four-vertices (17.4) are then recovered, in the partition function (17.5), from the diagrams



(17.11)

An important point to observe now is that the action (17.5) is quadratic in ϕ such that we can perform the Gaussian functional integral over ϕ using formula (10.24), obtaining

$$Z[j]=\mathcal{N}\int\mathcal{D}\sigma e^{i\int d^4x\left\{\frac{1}{4g}\sigma^2+iN\frac{\hbar}{2}\mathrm{Tr}\log\left(-\partial^2-m_0^2-\sigma\right)+\frac{i}{2}j\frac{i}{-\partial^2-m_0^2-\sigma}j\right\}}, \tag{17.12}$$

where the last term is due to the quadratic completion.[2]

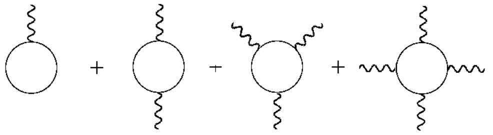
quadratic completion

The factor N in front of the trace log arises from the N components ϕ_a each of them giving the same contribution.

The new representation of $Z[j]$ describes the same physics in terms of a single composite field σ rather than N fundamental fields ϕ_a.

Since the main application of this formalism will be in many-body problems where composite fields describe collective phenomena, the field σ will be referred to as *collective field* and the exponent in (17.12) as *collective action.*

Let us derive the Feynman rules for the collective field theory. The "free part" of the action is $\sigma^2/4g$ with the σ-"propagator" (17.10). The vertices are obtained from the powers σ^n in an expansion of the remaining part of the collective action. The trace of the logarithm may be expanded into loops just as shown in (14.32). In contrast to the diagrams (14.36), the loops now emit single wiggly lines for σ rather than pairs of ϕ-lines



(17.13)

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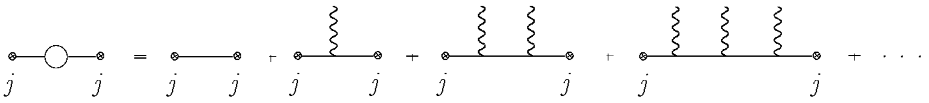
[2] In this context, the functional Gaussian Integral is called *Hubbard-Stratonovich transformation.* See R.L. Stratonovich, Sov. Phys. Dokl. **2**, 416 (1958); J. Hubbard, Phys. Rev. Letters **3**, 77 (1959); B. Mühlschlegel, J. Math. Phys. , **3**, 522 (1962); J. Langer, Phys. Rev. A **134**, 553 (1964); T.M. Rice, Phys. Rev. A **140** 1889 (1965); J. Math. Phys. **8**, 1581 (1967); A.V. Svidzinskij, Teor. Mat. Fiz. **9**, 273 (1971); D. Sherrington, J. Phys. C **4**, 401 (1971).

Similarly, the current piece may be expanded in σ as

$$-\frac{1}{2}j\frac{i}{-\partial^2-m_0^2-\sigma}j = -\frac{1}{2}j\left[\frac{i}{-\partial^2-m_0^2}+\frac{i}{-\partial^2-m_0^2}(-i\sigma)\frac{i}{-\partial^2-m_0^2}\right.$$
$$\left.+\frac{i}{-\partial^2-m_0^2}(-i\sigma)\frac{i}{-\partial^2-m_0^2}(-i\sigma)\frac{i}{-\partial^2-m_0^2}+\dots\right]. \tag{17.14}$$

This corresponds to the following Feynman graphs



(17.15)

(17.16)

in which a line connects two currents and emits any number of wiggly σ-lines along the way.

It is obvious that every fundamental graph can be recovered by connecting the σ-ends in (17.13) and (17.15) via the "propagator" $G_{\sigma\sigma} = 2g$.

17.2 The Limit of Large N

One of the most interesting features of the collective field theory is that it can be used to *solve* the full quantum field theory in the limit $N \to \infty$ if the coupling constnat is simultaneously decreased as $1/N$ by setting

$$g = g_1/N. \tag{17.17}$$

with fixed g_1, in order to see how this works we first rewrite, in the absence of external currents j the functional integral over σ as[3]

$$e^{iN\mathcal{A}_{\rm coll}[\sigma]} = \int \mathcal{D}\sigma e^{iN\int d^4x\left[\frac{1}{2g_1}\sigma^2 - i\frac{\hbar}{2}{\rm Tr}\log(-\partial^2-m_0^2-\sigma)\right]}. \tag{17.18}$$

But the factor N in the exponent has the same effect as previously $1/\hbar$ in the semiclassical limit. For $N \to \infty$, the exponential becomes a δ-functional around the extremum of the action which is given by

$$\Sigma(x) = 4g_1\frac{\hbar}{2}\left(\frac{i}{-\partial^2-m_0^2-\Sigma}\right)(x,x). \tag{17.19}$$

Fluctuations around this solution are suppressed by a factor $1/N$ (just as previously $\hbar$). Thus, to leading order in N, the generating functional is given by

$$W[j]|_{j=0} = \mathcal{A}_{\rm coll}[\Sigma] = \int d^4x\left[\frac{1}{2g}\Sigma^2 - iN\frac{\hbar}{2}{\rm Tr}\log(-\partial^2-m_0^2-\Sigma)\right].$$

---

[3] K. Wilson, Phys. Rev. D 7, 2911 (1973)

Let us now include external currents and consider

$$e^{iW[j]} = \int \mathcal{D}\sigma \exp\left\{iN\mathcal{A}_{\rm coll}[\sigma] - \frac{1}{2}j\frac{i}{-\partial^2 - m_0^2 - \sigma}j\right\}. \tag{17.20}$$

Then as $N \to \infty$, we have to allow for the possibility that the external particles contribute to leading order in N (for instance if there is one external line for each index $a = 1, \dots, N$). Then the field σ has to be chosen to extremize the full exponent which happens, say at $\sigma = \Sigma[j]$. The extremization becomes more familiar looking by going from $W[j]$ to the effective action. For this we introduce the effective field

$$\Phi_a[j] = \frac{\delta W[j]}{\delta j_a} = i\frac{i}{-\partial^2 - m_0^2 - \Sigma[j]}j_a, \tag{17.21}$$

whose inversion yields $j_a = j_a[\Phi_a]$ and from this $\Sigma[\Phi] = \Sigma[j[\Phi]]$. Note that there is no contribution from the $\delta\Sigma/\delta j_a$-dependence via the chain rule $\delta\Sigma/\delta j_a \delta W[j]/\delta\Sigma$, since $W[j]$ is extremal in Σ for fixed j_a. Now we may calculate the effective action from

$$\Gamma[\Phi] \;=\; N\mathcal{A}_{\rm coll}[\Sigma] - \frac{1}{2}\int d^4x \Phi_a\left\{-\partial^2 - m_0^2 - \Sigma\right\}\Phi_a - j_a[\Phi_a]\Phi_a. \tag{17.22}$$

Here Σ is the extremal functional $\Sigma[\Phi]$, It is obvious that this functional can be obtained directly from minimizing (17.22) at a constant Φ. This is so since the extremality condition

$$K = \frac{\delta W[j]}{\delta\Sigma} = 0$$

determines $\Sigma = \Sigma[j]$, and implies also that

$$\Gamma_\Sigma[\Phi] = [W[j] - \Phi j]_\Sigma = \left(W_j[j] - \Phi\right) j_\Sigma + W_\Sigma[j] = 0, \tag{17.23}$$

a relation which serves to determine $\Sigma = \Sigma[\Phi]$. Thus it is more practical to consider

$$\Gamma[\Phi, \Sigma] = N\mathcal{A}_{\rm coll}[\Sigma] + \frac{1}{2}\int d^4x\, \Phi_a \left(-\partial^2 - m_0^2 - \Sigma\right) \Phi_a \tag{17.24}$$

as an effective action of two fields Φ and Σ. The physical field configurations are obtained by extremizing $\Gamma[\Phi, K]$ with respect to *both* arguments, thus obtaining say, Φ^0, Σ^0.

The calculation of higher vertex functions proceeds as follows. One expands $\Gamma[\Phi, \Sigma]$ around Φ^0, Σ^0 by writing

$$\begin{aligned} \Gamma[\Phi, \Sigma] \;&=\; \Gamma\left[\Phi^0 + \Phi', \Sigma^0 + \Sigma'\right] = \Gamma\left[\Phi^0, \Sigma^0\right] \\ &+\; \frac{1}{2}\left\{\Gamma_{\Phi\Phi}\left[\Phi^0, \Sigma^0\right]\Phi'\Phi' + 2\Gamma_{\Sigma\Phi}\left[\Phi^0\Sigma^0\right]\Phi'\Sigma' + \Gamma_{\Sigma\Sigma}\left[\Phi^0\Sigma^0\right]\Sigma'\Sigma'\right\} \\ &+\; \text{higher derivative terms.} \end{aligned} \tag{17.25}$$

This first derivatives vanish, the second determine propagators of Φ' and Σ' fields

$$G_{\Phi'\Phi'} = i\Gamma^{-1}_{\Phi\Phi}\left[\Phi^0, \Sigma^0\right] \tag{17.26}$$

$$G_{\Sigma'\Sigma'} = i\Gamma^{-1}_{\Sigma\Sigma}\left[\Phi^0, \Sigma^0\right]. \tag{17.27}$$

By means of the vertex functions fixed by the higher derivatives we may now compose all tree diagrams. Only those with external Φ' lines survive since $\Gamma_\Sigma = 0$. But any number of internal Σ'-lines may occur.

Let us convince ourselves that these vertex functions are the same as those which would be obtained from higher functional derivatives of $\Gamma[\Phi]$ of (17.22). In order to avoid writing the two arguments of $\Gamma\left[\Phi, \Sigma\right]$ let us denote $\Gamma[\Phi] \equiv \Gamma\left[\Phi, \Sigma[\Phi]\right]$ by $F[\Phi]$ for the discussion to follow, i.e.,

$$F[\Phi] \equiv \Gamma\left[\Phi, \Sigma[\Phi]\right] \tag{17.28}$$

As argued before, the functional $\Sigma[\Phi]$ satisfies

$$\Gamma_\Sigma\left[\Phi, \Sigma[\Phi]\right] = 0 \tag{17.29}$$

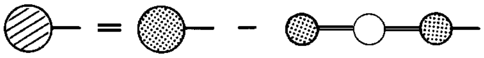
or

$$\Sigma_\Phi = -\Gamma^{-1}_{\Sigma\Sigma}\Gamma_{\Sigma\Phi}. \tag{17.30}$$

This relation can be used when deriving the higher vertex functions from (17.28):

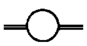
$$F_\Phi = \Gamma_\Phi + \Gamma_\Sigma \Sigma_\Phi = \Gamma_\Phi - \Gamma_\Sigma \Gamma^{-1}_{\Sigma\Sigma}\Gamma_{\Sigma\Phi}. \tag{17.31}$$

This may be represented graphically as



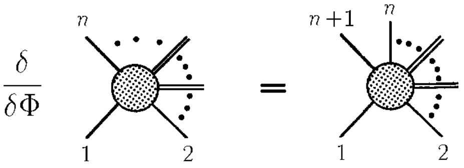
(17.32)

An open blob with two double legs stands for the second functional derivative of $\Gamma[\Sigma, \Phi]$ with respect to Σ, which is $-i$ times the propagator of the Σ'-field:



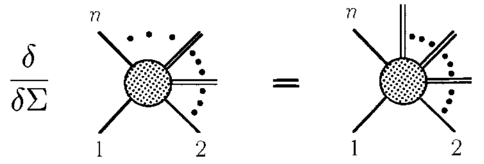
$$= \Gamma^{-1}_{\Sigma\Sigma} = -i\,\dot{\Sigma}'\dot{\Sigma}'. \tag{17.33}$$

The grey blobs are the vertices of the two-argument effective action $\Gamma\left[\Phi, \Sigma\right]$. They have single or double legs emerging, the latter representing the Σ'-field. Differentiation this with respect to Φ adds one more single leg:



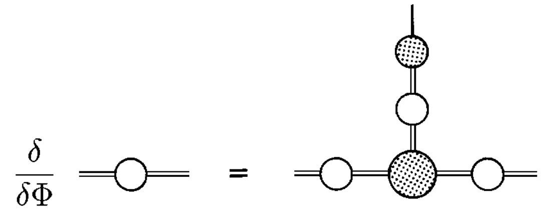
(17.34)

A differentiation with respect to Σ adds one more double leg:



(17.35)

Since $\delta\Gamma^{-1}_{\Sigma\Sigma}/\delta\Phi = \Gamma^{-3}_{\Sigma\Sigma}\Gamma_{\Sigma\Phi}$ we see that differentiating (17.33) with respect to Φ produces a three-Σ' vertex:

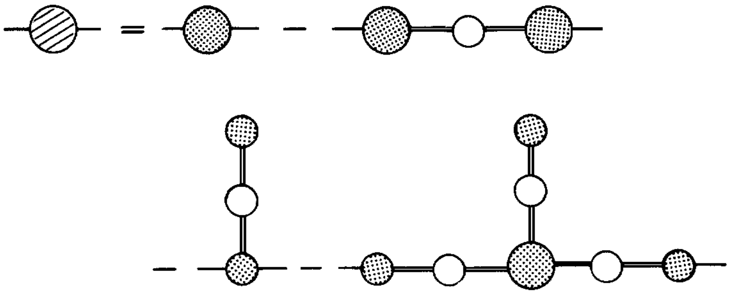


(17.36)

Differentiating (17.31) further we find

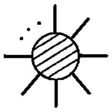
$$F_{\Phi\Phi} = \Gamma_{\Phi\Phi} - \Gamma_{\Phi\Phi}\Gamma^{-1}_{\Sigma\Sigma}\Gamma_{\Sigma\Phi} - \Gamma_{\Sigma}\Gamma^{-1}_{\Sigma\Sigma}\Gamma_{\Sigma\Phi\Phi} - \Gamma_{\Phi\Sigma}\Gamma^{-3}_{\Sigma\Sigma}\Gamma_{\Sigma\Sigma\Sigma}\Gamma_{\Sigma\Phi}\Gamma_{\Sigma} \tag{17.37}$$

which has the graphical form

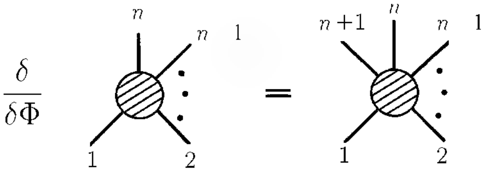


(17.38)

The procedure can be continued via the chain rule of differentiation. A blob with n legs

$F_{\Phi\Phi\ldots\Phi} =$  (17.39)

represents an n-point vertex function $F_{\Phi\Phi\ldots\Phi}$. A differentiation with respect to the field Φ adds, step by step, one more external leg, i.e.,



(17.40)

Proceeding in this way we can keep on differentiating (17.37) and construct all higher diagrams. At the end, we discard all diagrams in which a double line ends in a shaded blob (Σ-line tadpole diagrams), since Σ is extremal such that $\Gamma_\Sigma = 0$. The particular structure of $\Gamma[\Phi, \Sigma]$ in Eq. (17.24)

$$\Gamma[\Phi, \Sigma] = N\mathcal{A}_{\rm coll}[\Sigma] + \frac{1}{2}\int d^4x \Phi_a \left(-\partial^2 - m_0^2 - \Sigma\right)\Phi_a \qquad (17.41)$$

can be used to simplify these graphical rules. If we set $\gamma[\Sigma] \equiv N\mathcal{A}_{\rm coll}[\Sigma]$, we obtain the simple vertex functions

$$\begin{aligned}
\Gamma_{\Phi_a\Phi_b} &= \left(-\partial^2 - m_0^2 - \Sigma\right)\delta_{ab} && (17.42)\\
\Gamma_{\Sigma\Phi_a} &= -\Phi_a, && (17.43)\\
\Gamma_{\Sigma\Phi_a\Phi_b} &= -\delta_{ab}, && (17.44)\\
\Gamma_{\Sigma\Phi_{a_1}\dots\Phi_{a_n}} &= 0, \qquad n \geq 2, && (17.45)\\
\Gamma_{\Sigma_1\dots\Sigma_n\Phi_a} &= 0, \qquad n \geq 2, && (17.46)\\
\Gamma_{\Sigma_1\dots\Sigma_n} &= \gamma_{\Sigma_1\dots\Sigma_n} \qquad n \geq 2. && (17.47)
\end{aligned}$$

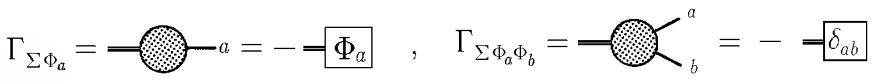
Then (17.37) becomes

$$\Gamma_{\Phi_a\Phi_b} = -\partial^2 - m_0^2 - \Sigma - \Phi_a\gamma^{-1}_{\Sigma\Sigma}\Phi_b + \Gamma_\Sigma\gamma^{-1}_{\Sigma\Sigma} - \Gamma^{-3}_{\Sigma\Sigma}\gamma_{\Sigma\Sigma\Sigma}\Phi^2\Gamma_\Sigma. \qquad (17.48)$$

This has to be evaluated at the extremum where $\Gamma_\Sigma = 0$. We therefore obtain the propagator of the Φ-field

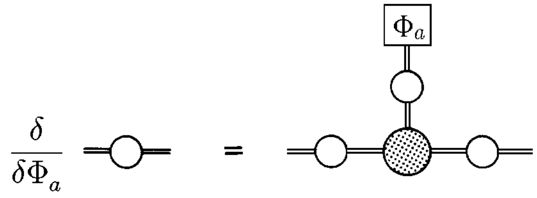
$$G = iF^{-1}_{\Phi\Phi} = i\left[\left(-\partial^2 - m_0^2 - \Sigma\right)\delta_{ab} - \Phi_a\gamma^{-1}_{\Sigma\Sigma}\Phi_b\right]^{-1}. \qquad (17.49)$$

Graphically, we exhibit the simplification brought about by Eq. (17.42) and (17.43) by replacing the diagrams $\Gamma_{\Sigma\Phi}$ and $\Gamma_{\Sigma\Phi\Phi}$ as follows:



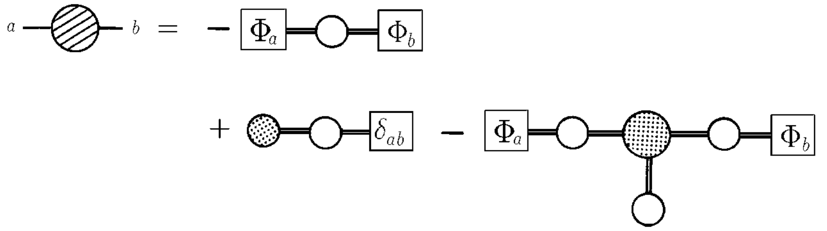
(17.50)

Then (17.36) looks as follows:



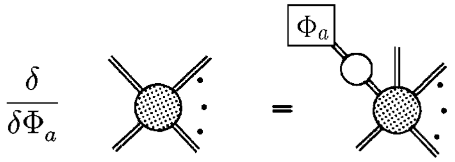
(17.51)

and (17.38):



(17.52)

A functional differentiation of $\Gamma_{\Sigma\Sigma\cdots\Sigma}$ with more than one Σ-leg with respect to Φ gives



(17.53)

Let us finally write down the propagators and vertices of the Σ'-field explicitly. For this we consider the Taylor series of the trace log term in (17.18):

$$
\begin{aligned}
&N\frac{i}{2}\mathrm{Tr}\log\left(-\partial^2-m_0^2-\Sigma^0-\Sigma'\right)\\
&= N\frac{i}{2}\left[\mathrm{Tr}\log\left(-\partial^2-m_0^2-\Sigma^0\right)+\mathrm{Tr}\log\left(1+\frac{i}{-\partial^2-m_0^2-\Sigma^0}i\Sigma'\right)\right]\\
&= N\frac{i}{2}\sum_{n=1}^{\infty}\frac{1}{n}\left[\frac{i}{-\partial^2-m_0^2-\Sigma^0}\left(-i\Sigma'\right)\right]^n . \qquad (17.54)
\end{aligned}
$$

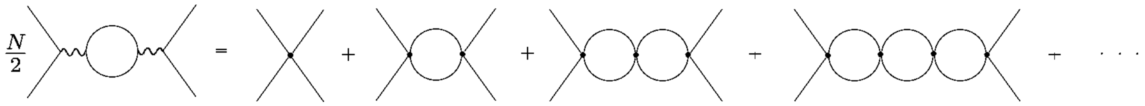
Reading off the quadratic terms

$$
\frac{N}{4}\left[\frac{1}{g_1}\Sigma'^2+i\mathrm{Tr}\left(\frac{i}{-\partial^2-m_0^2-\Sigma^0}\Sigma'\right)\right], \qquad (17.55)
$$

we find in momentum space the Wick rotated propagator

$$
G_{\Sigma'\Sigma'}(q')\equiv i\Gamma^{-1}_{\Sigma\Sigma}=\delta^{(4)}(q-q')\frac{2}{N}i\left\{\frac{1}{g_1}\int\frac{d^Dk}{(2\pi)^D}\frac{1}{k^2-m_0^2-\Sigma^0}\,\frac{1}{(q-k)^2-m_0^2-\Sigma^0}\right\}^{-1}. \qquad (17.56)
$$

This propagator is a non-perturbative object. Expanding it in powers of g_1, we may write the interaction caused by it as a series of ordinary Feynman diagrams



(17.57)

where the wiggle with a blub represents the propagator (17.56) of the Σ'-field, a line the simple Φ' propagator

$$G_{\Phi'\Phi'} = \frac{i}{-\partial^2 - m_0^2 - \Sigma^0}, \tag{17.58}$$

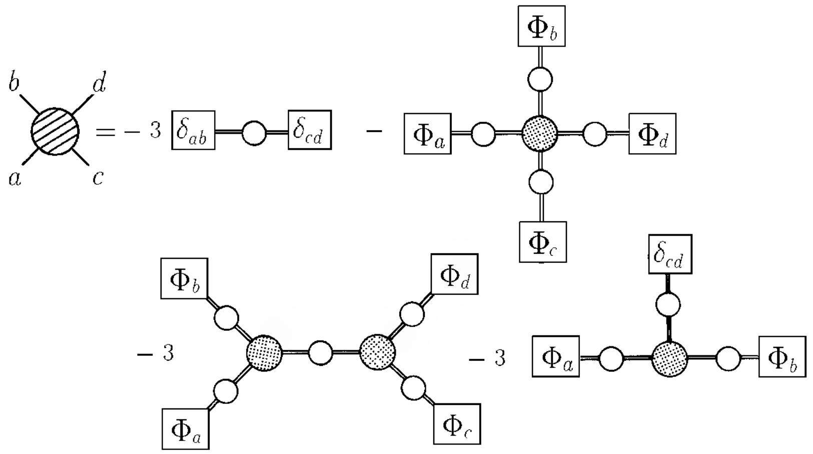
and a dot the fundamental ϕ^4-vertex g_1.

It should be pointed out that the higher terms bubble sum in (17.57) do not carry the same multiplicity factors as in the original perturbation expansion of the ϕ^4-theory in (8.6.1). The factors in that expanson are $4g/4!$, $(4!4!/2)(g/4!)^2$ for zero- and one-bubble diagrams. After exchanging $g/4! \to g/4$ these become $6g$, $24g^2$. In the σ exchange between two Φ'-lines, only only one third of the contractions are done, so that $6g$ goes reduces to $2g = 2g_1/N$, which explains the first term in the propagator (17.57). For N components, the second multiplicity receives a factor $T_I = (N+8)/9$ [recall (9.224) and (9.233)], which in the limit $N \to \infty$ becomes $N/9$. Thus the second terms carries a factor $2Ng^2 = 2g_1/N$, in agreement with the second term in (17.57).

The n-point vertex functions for the Σ' field are given by

$$-\frac{N}{2} i \frac{i}{n} \left[\frac{i}{-\partial^2 - m_0^2 - \Sigma^0} \left(-i\Sigma' \right) \right]^n \tag{17.59}$$

which are the one-loop diagrams (17.13) with Φ' lines emerging from the cirle. In this way every n-point vertex function of the original field theory has been reduced, in the limit $N \to \infty$, to a finite sum of tree diagrams involving Σ' propagators and Σ'-vertices, all of which consist of one-loop diagrams of the Φ' field. For the four-point function we obtain



(17.60)

plus terms which contain Γ_Σ at the end of one double line and vanish at the extremum. We now see that the rules derived in this algebraic fashion are indeed just the Feynman rules for the tree diagrams of the theory with propagators

$$G_{\Sigma'\Sigma'} = i\gamma^{-1}_{\Sigma\Sigma}$$

and shaded blobs as vertices representing $\gamma_{\Sigma\Sigma\cdot\Sigma}$. The double lines may either end in a field Φ_a or in a Kronecker δ_{ab}.

17.3 Variational Equations

We have seen in Section 12.9 that the effective action can be used as a basis for variational calculations of a field theory. As an application we study here a simple exactly solvable field-theoretic model which permits us to see the effect of all loop corrections. The simplest model is a ϕ_a^4-theory with N fields $\phi_1, \ldots, \phi_N$ in the limit $N \to \infty$. In statistical mechanics, this is known as the *spherical model.* In the last section, we we have derived the effective action as a function of the classical field $\Phi_a(x)$ and the collective field $\Sigma(x)$ as

$$\begin{aligned}\Gamma\left[\Phi_a, \Sigma\right] = \mathcal{A}[\Phi_a] + \Gamma_{\rm coll}\left[\Phi, \Sigma\right] &= \int d^D x \left[\frac{1}{2}\left(\partial\Phi_a\right)^2 - \frac{m_0^2}{2}\Phi_a^2 - \frac{1}{2}\Sigma\,\Phi_a^2 + \frac{N}{4g_0}\Sigma^2\right] \\ &+ \frac{i}{2} N \,{\rm Tr}\log\left(-\partial^2 - m_0^2 - \Sigma\right). \qquad (17.61)\end{aligned}$$

To leading order in N, this is the exact effective action of the theory. For the discussion to follow it will be useful to abbreviate $m_0^2 + \Sigma(x)$ by $\lambda(x)$:

$$m_0^2 + \Sigma(x) \equiv \lambda(x), \qquad (17.62)$$

since this combination appears inside the functional Tr log like a spacetime-dependent mass term. Then we write

$$\begin{aligned}\Gamma\left[\Phi_a, \lambda\right] &= \int d^D x \left[\frac{1}{2}\left(\partial\Phi_a\right)^2 - \frac{1}{2}\lambda\Phi_a^2 - \frac{N}{2g_0} m_0^2 \lambda + \frac{N}{4g_0}\lambda^2 + \frac{N}{4g_0} m_0^4\right] \\ &+ + \frac{i}{2} N \,{\rm Tr}\log\left(-\partial^2 - \lambda\right). \qquad (17.63)\end{aligned}$$

According to Eq. (12.79), the effective action has to be extremal for physical values of the vacuum expectation of the fields $\Phi_a = \langle\phi_a\rangle$. We expect the ground state to be isotropic in spacetime, and look for minima of the effective potential as a function of *constant* fields λ, Φ_a, for which the functional Tr log reduces to a simple integral over phase space. Dividing out the spacetime volume, we obtain the effective potential

$$v(\Phi, \lambda) = \frac{1}{2}\lambda\Phi_a^2 + \frac{N}{2g_0} m_0^2 \lambda - \frac{N}{4g_0}\lambda^2 - \frac{N}{4g_0} m_0^4 + \frac{N}{2}\int \frac{d^D k}{(2\pi)^D} \log\left(k^2 + \lambda\right). \qquad (17.64)$$

The momentum integral can be done using formula (9.133) and we obtain

$$v(\Phi, \lambda) = \frac{1}{2}\lambda\Phi_a^2 + \frac{N}{2g_0} m_0^2 \lambda - \frac{N}{4g_0}\lambda^2 - \frac{N}{4g_0} m_0^4 + \frac{1}{2} N S_D \frac{1}{2}\Gamma(D/2)\Gamma(1 - D/2)\frac{2}{D}\lambda^{D/2}. \qquad (17.65)$$

To find the extrema of this we distinguish two cases:

1. $$\frac{\partial V}{\partial \Phi_a} = \lambda \Phi_a = 0, \tag{17.66}$$

which allows for the two possible solutions:

a) $\Phi_a = 0$,

b) $\Phi_a \neq 0, \quad \lambda = 0.$

2. $$\frac{\partial V}{\partial \lambda} = \Phi_a^2 + \frac{Nm_0^2}{g_0} - \frac{N}{g_0}\lambda + NS_D \frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\lambda^{D/2-1} = 0. \tag{17.67}$$

The extremum 1a) corresponds to a normal ground state possessing the same O(N)-symmetry as the original action. The ground state associated with the other extremum 1b), on the other hand, breaks the O(N)-symmetry of the action. This phenomenon is called *spontaneous symmetry breakdown*. It is a universal phenomenon in many-body systems, where it is observed in the form of ordered phases. The most widely known systems of this type are ferromagnets, which display a spontaneous magnetization sufficiently low temperature. The magnetization vector may be identified with the field at an expectation Φ_a for $N = 3$. The magnetized state is not rotationally invariant, and violates the rotational invariance of the Hamilton operator of the system. Above a critical temperature called *Curie* or *Néel temperature*, the system looses its magnetization and becomes rotationally symmetric. This is the normal state.

In the O(N)-symmetric solution 1a), the second equation (17.67) determines λ:

$$\frac{Nm_0^2}{g_0} = \frac{N}{g_0}\lambda - NS_D \frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\lambda^{D/2-1}. \tag{17.68}$$

In the case 1b), it determines

$$\Phi_a^2 = -\frac{Nm_0^2}{g_0}. \tag{17.69}$$

We have seen before that the functional integral is stable only for $g_0 > 0$. The state with spontaneously broken O(N)-symmetry can exist only for ${m_0}^2 < 0$.

17.3.1 Non-trivial Ground States

The solutions to the above equations depend on the dimension of spacetime, and will therefore be discussed separately:

Dimension D=4

Setting $D = 4 - \epsilon$ and using (9.160) to expand

$$\frac{1}{2}\Gamma(D/2)\Gamma(1-D/2) = -\frac{1}{\epsilon} + \mathcal{O}(\epsilon),$$

equation (17.67) becomes

$$\Phi_a^2 = \frac{N}{g_0}\left(\lambda - m_0^2\right) + NS_D\mu^{-\epsilon}\lambda\frac{1}{\epsilon} - NS_D\mu^{-\epsilon}\lambda\log\frac{\lambda}{\mu^2}. \tag{17.70}$$

This is renormalized by introducing the physical masses and coupling constants m and g:

$$\frac{1}{g} \equiv \frac{1}{g_0\mu^\epsilon} + S_D\frac{1}{\epsilon}, \tag{17.71}$$

$$\frac{m^2}{g} = \frac{m_0^2}{g_0}, \tag{17.72}$$

with an arbitrary mass parameter μ. Then we can take the limit $\varepsilon \to 0$ in (17.70) and find

$$\Phi_a^2 = \frac{N}{g}\left(\lambda - m^2\right) - NS_4\frac{1}{2}\lambda\log\frac{\lambda}{\mu^2}. \tag{17.73}$$

where $S_4 = 1/8\pi^2$ the corresponding potential is

$$v(\Phi,\lambda) = \frac{1}{2}\lambda\Phi_a^2 + \frac{N}{2g}m^2\lambda - \frac{N}{4g}\lambda^2 - \frac{N}{4g_0}m_0^4 + NS_4\frac{1}{8}\lambda\left(\log\frac{\lambda}{\mu^2} - \frac{1}{2}\right). \tag{17.74}$$

Consider the ground state with a spontaneous symmetry breakdown, where the minimum of $n(\Phi_a, M)$ lies at $\Phi_a \neq 0$ with $\lambda = 0$. From (17.69) and (17.72), this minimum lies at

$$\Phi_a^2 = -\frac{Nm^2}{g} \tag{17.75}$$

For positive renormalized coupling constant g, this ground state requires a regular m^2. Let us see how $v(\Phi_a, M)$ behaves in the neighborhood of $m^2 = 0$. For $m^2 > 0$, Φ_a^2 necessarily increases since the logarithm in (17.74) is negative. Its slope in λ is initially infinite, being given by

$$\frac{\partial v(\Phi_a,\lambda)}{\partial\lambda} = \frac{1}{2}\left[\Phi_a^2 + \frac{Nm^2}{g} - \frac{N}{2g}\lambda - NS_4\frac{1}{4}\left(\log\frac{\lambda}{\mu^2} + \frac{1}{2}\right)\right]. \tag{17.76}$$

If we insert (17.73) back into the potential (17.74), we find

$$v_{\rm min} = \frac{1}{4}\lambda\left(\Phi_a^2 + \frac{Nm^2}{g}\right) - NS_4\frac{1}{16}\lambda^2. \tag{17.77}$$

Then, for increasing small λ, the potential increases. This goes on until $v_{\rm min}$ reaches a maximum which is determined by

$$\Phi^2_{a\,\rm max} + \frac{Nm^2}{g} = N S_4 \frac{1}{2}\lambda_{\rm max}. \tag{17.78}$$

Together with (17.73) this implies

$$\log\frac{\lambda_{\rm max}}{\mu^2} = -1 + \frac{2}{gS_4}. \tag{17.79}$$

If we want to calculate $\Phi_a(M)$ for a value $\Phi_a^2 > \Phi^2_{a\,\rm max}$, we have to choose λ complex, so that also the potential becomes complex indicating an instability of the corresponding state. Even though this field configuration can be reached only via an external current, there are disastrous consequences as we shall see later when discussing the Green functions of the theory.

A similar phenomenon arises for $\Phi_a^2 < -Nm^2/g$. Then Δ has to be taken imaginary (note: real negative Δ would give an imaginary Φ_a^2). Also there, $v(\Phi_a, \lambda)$ becomes complex. Contrary to the previous regime, however, this complexity is of a simple physical nature. We shall see in Section 15.2 that it is related to a singularity of all Green functions at zero energymomentum which arises from the massless Nambu-Goldstone bosons.

Dimension D=3

Here the equation (17.67) reads

$$\Phi_a^2 = \frac{N}{g_0}\left(m^2 - m_0^2\right) + N S_3 M, \tag{17.80}$$

where $S_3 = 1/2\pi^2$). With this regularization neither m_0^2 nor g_0 need to be renormalized, so that they can be replaced by m^2 and g. The potential becomes

$$v(\Phi_a, M) = \frac{1}{2}\left(\Phi_a^2 + \frac{Nm^2}{g}\right) - \frac{N}{4g}\lambda^2 - N S_3 \frac{\pi}{6}\lambda^{3/2}. \tag{17.81}$$

Again, as λ increases from zero, $\Phi_a^2 + Nm^2/g$ moves to positive values. The potential at the extremum g in λ is

$$\begin{aligned} v_{\rm ext} &= \lambda\left(\Phi_a^2 + \frac{Nm^2}{g}\right)\left(\frac{1}{2} - \frac{1}{D}\right) - \frac{N}{4g}\left(1 - \frac{4}{D}\right)\lambda^2 \\ &= \frac{1}{6}\lambda\left(\Phi_a^2 + \frac{Nm^2}{g}\right) + \frac{1}{12}\frac{N}{g}\lambda^2 \end{aligned} \tag{17.82}$$

There is now an important difference with respect to the previous $D = 4$, case. The potential increases monotonously for $\Phi_a^2 > -Nm^2/g$ and does not become complex for any large positive Φ^2. For $\Phi_a^2 < -Nm^2/g$, however, the situation is in some respect similar to $D=4$, but in an important respect it is different. To see most easily what happens we may express λ from (17.67) in terms of $\Phi_a^2 + Nm^2/g$ and have

$$\sqrt{\lambda} = -\frac{g}{4} S_3 \pi + \left[\left(\frac{g S_3 \pi}{4} \right)^2 + \frac{g}{N} \left(\Phi_a^2 + \frac{Nm^2}{g} \right) \right]. \tag{17.83}$$

As long as $\Phi_a^2 > -Nm^2/g$, the solution has $\sqrt{\lambda} > 0$. Below this value, the square root becomes negative. Thus there is again a complex value of the auxiliary field λ, just as for $D=4$. The difference with respect to that case lies in the fact that in spite of λ being complex $v(\Phi_a, \lambda)$ remains real, and increases with $\Phi^2 < -Nm^2/g$. It therefore has a proper minimum at $\Phi^2 = -Nm^2/g$. Thus the theory is consistent and displays a spontaneous breakdown of $O(N)$-symmetry.

Dimension D=2

In two dimensions everything changes drastically. Here the potential becomes for $D = 2+\epsilon$ [using $\Gamma(D/2)\Gamma(1-D/2)2/D \approx -2/\epsilon + 1$]

$$V \;=\; \frac{1}{2}\lambda\Phi_a^2 + \frac{N}{2g_0} m_0^2 \lambda - \frac{N}{4g_0}\lambda^2 - -\frac{N}{4g_0} m_0^4 - \frac{1}{4} N S_2 \lambda \left(\log \frac{\lambda}{\nu^2} - 1 \right),$$

so that Eq. (17.67) becomes

$$\Phi_a^2 = \frac{N}{g_0}\left(\lambda - m_0^2\right) + N S_D \frac{1}{\epsilon} + \frac{1}{2} N \mu^2 S_D \log \frac{\lambda}{\mu^2}. \tag{17.84}$$

We can again renormalize the mass by introducing

$$m^2 = m_0^2 - g_0 S_D \frac{1}{\epsilon}. \tag{17.85}$$

For the coupling constant there is no need of renormalization, i.e., $g = g_0$. Then the finite equation reads

$$\Phi_a^2 = \frac{N}{g}\left(\lambda - m^2\right) + \frac{1}{2} N S_2 \log \lambda/\mu^2 \tag{17.86}$$

where $S_2 = 1/2\pi$. The potential at the minimum is given by

$$v_{\rm min} \;=\; \frac{1}{2}\lambda\left(\Phi^2 + \frac{Nm^2}{g}\right) - \frac{N}{4g}\lambda^2 + N\frac{1}{4} S_2 \lambda \left(\log \lambda/\mu^2 - 1\right). \tag{17.87}$$

Now Φ_a^2 as a function of λ behaves quite different from the previous cases. There is no finite value of Φ_a^2 for which λ can be equal to zero since for $\lambda \to 0, \Phi_a^2$ to $-\infty$. Thus there can be no spontaneous symmetry breakdown in two dimensions. This condensation turns out to have an exception for $N=2$, where there exists a quasi-ordered ground state with a quasi-symmetry breakdown. The conclusion also does not apply to $N=1$. Since the $O(1)$ symmetry is discrete, the only group elements being 1 and -1. The O(1)-symmetric ϕ^4-theory is equivalent to an Ising model of magnetism which is well-known to have a second-order phase transition into a magnetized state, which is a phase with broken symmetry.

Dimension D=1

Also in one dimension, there can be no spontaneous symmetry breakdown. This is obvious since the system is equivalent, to quantum mechanics of a particle at the time dependent position $\phi(t)$, i.e., the Hamiltonian

$$H = \frac{1}{2}\left(\partial\phi_a\right)^2 - \frac{m_0^2}{2}\phi_a^2 - \frac{g_0}{4N}\left(\phi_a^2\right)^2 \tag{17.88}$$

may be interpreted as that of a mass point in N-dimensional space moving in an $O(N)$-invariant potential. The ground state is unique, and there can be no degeneracy, hence no spontaneous symmetry breakdown. Contrary to the case $D = 2$, this argument also holds for any N, also for $N = 2$ and $N = 1$. Certainly, Eq. (17.67) has to reflect this feature and it indeed does so. There is now no need for renormalization and, so that we can omit the subscripts zero and find for $D = 1$ with $\bar{S}_1 = 1/\pi$:

$$\Phi_a^2 = \frac{N}{g}\left(\lambda - m^2\right) - (\lambda)^{-1/2}, \tag{17.89}$$

$$v_{\text{min}} = -\frac{1}{2}\lambda\left(\Phi^2 + \frac{Nm^2}{g}\right) + \frac{N}{4g}\lambda^2. \tag{17.90}$$

Again there is no solution for $\lambda \to 0$, since this would imply $\Phi_a^2 \to -\infty$.

17.4 Special Features of Two Dimensions

The impossibility of the spontaneous breakdown of a continous symmetry in two spacetime dimensions is related to the fact such a phase would contain massless Nambu-Goldstone bosons in two dimensions. But it can be shown that massless fields $\phi(x)$ cannot exist in this reduced spacetime. The reason is basically, that the associated propagator

$$G(x) = \langle\phi(x)\phi(0)\rangle = \int \frac{d^2q}{(2\pi)^2}\frac{i}{q^2}e^{iqx} \tag{17.91}$$

is divergent for all $\mathbf{x}$, due to the singularity at $q = 0$. It needs a small-q cutoff, or equivalently an infinitesimally small mass μ. In D dimensions, the massive propagator reads, according to (5.135) Eq. (5.133),

$$\begin{aligned} G(x) &= \int \frac{d^Dq}{(2\pi)^D}\frac{i}{q^2-\mu^2}e^{iqx} \\ &= \frac{1}{(2\pi)^{D/2}}\left(\frac{\mu}{|x|}\right)^{D/2-1} K_{D/2-1}(\mu|x|). \end{aligned} \tag{17.92}$$

where $|x| \equiv \sqrt{-(x-x')^2}$. For $|x| \ll 1/\mu$, which due to the smallness of μ is almost no restriction, we use the small-argument limit of the Bessel function

$$K_\nu(z) \approx \Gamma(\nu)\frac{1}{2}\left(\frac{2}{z}\right)^\nu, \tag{17.93}$$

to obtain the approximations

$$G(x) \approx \begin{cases} \Gamma(D/2-1)\dfrac{1}{4\pi^{D/2}|x|^{D-2}}, & D>2 \\ -\dfrac{1}{2\pi}\log\dfrac{\mu\sqrt{-x^2}}{2e^{-\gamma}}, & D=2. \end{cases} \tag{17.94}$$

where $\gamma = 0.577\dots$ is Euler's number. The two-dimensional expression diverges in the limit $\mu \to 0$. This behavior has given rise to a physical feature of two-dimensional systems, formulated as a theorem, which in many-body physics is known as the *Mermin-Wagner theorem*, and in qunatum field theory as *Coleman's theorem*.[4]

Nonwithstanding this theorem, the system in which one would have expected massless Nambu-Goldstone modes do have a characteristic feature: They show what are called *quasi-long-range correlations*. These lead to physical observations which are quite similar to those of proper long-range fluctuations.[5] There are experiments which measure correlation functions of the exponential of such fields, and these have a power-like behavior. Let us calculate this. By Eq. (17.94) we have

$$\begin{aligned} C(x) \equiv \left\langle e^{ia\phi(x)}e^{-ib\phi(0)}\right\rangle &= e^{-\frac{1}{2}\langle[a\phi(x)-b\phi(0)]^2\rangle} = e^{-\frac{1}{2}\langle a^2\phi^2(x)-2ab\phi(x)\phi(0)+b^2\phi^2(0)\rangle} \\ &= e^{-\frac{1}{2}(a-b)^2G(0)}e^{ab[G(x)-G(0)]}. \end{aligned} \tag{17.95}$$

Now, since $G(0)$ is positively infinite, the prefactor vanishes unless $a=b$, in which case it is equal to unity, and we obtain

$$\left\langle e^{ia\phi(x)}e^{-ia\phi(0)}\right\rangle = e^{-\frac{a^2}{2}\langle[\phi(x)-\phi(0)]^2\rangle} = e^{a^2[G(x)-G(0)]}. \tag{17.96}$$

The exponent contains now the subtracted propagator (17.94):

$$G'(x) \equiv G(x)-G(0) \equiv \int \frac{d^2q}{(2\pi)^2}\frac{i}{q^2-\mu^2}\left(e^{iqx}-1\right) \approx -\frac{1}{2\pi}\log\frac{\Lambda\sqrt{-x^2}}{2e^{-\gamma}}. \tag{17.97}$$

In contrast to (17.94), this subtracted integral is now infrared finite but ultraviolet-divergent, and contains therefore an ultraviolet cutoff Λ. The x-behavior (17.97) is correct for $|x| \gg 1/\Lambda$, which is again almost everyhwere, due to the large size of Λ.

After inserting (17.97) into the correlation function (17.95) with $a=b$, we obtain the pure power falloff behavior with the distance

$$C(x) = \left(\frac{\Lambda\sqrt{-x^2}}{2e^{-\gamma}}\right)^{-a^2/2\pi}, \tag{17.98}$$

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[4] D. Mermin and H. Wagner, Phys. Rev. Lett. *22*, 1133 (1966); S. Coleman, Comm. Math. Phys. *31*, 259 (1973).

[5] For more details see H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I Superflow and Vortex Lines, World Scientific, Singapore 1989, pp. 1–744.

called *quasi-long-range behavior*. It is observed experimentally for many observables in two-dimensional systems where a perfectly ordered stae is forbidden by the Mermin-Wagner theorem.

In two dimensions, the system with the complex pair field Δ exhibits also a completely new pheomenon. There are macroscopic quantum fluctuations which produce quantum vortices and antivortices, in analogy to the vortex lines in three-dimensional superfluid helium and superconductors, discussed in Section ??. They attract each other by a logarithmic potential just like an electron gas with Coulomb interaction. At a temperature T_c, the long-range correlations of this Coulomb interaction is made short range by screening, which is caused by the dissociation of vortex pairs into free vortices. Thus there is a phase transition even though there can be no condensate.[6]

17.5 Experimental Consequences

Given the effective potentials and the associated ground states and assuming that the $N \to \infty$ limit carries valid information also for finite N we can study the radiative correction to field expectation values like

$$\langle \phi^2(x) \rangle \tag{17.99}$$

and the susceptibility

$$\begin{aligned} (2\pi)^D \delta^{(D)}(q+q')\chi^{-1}(q) &\equiv \langle T\phi_a(q)\phi_b(q')\rangle_{\rm c} \\ &= - \left.\frac{\delta^2\Gamma[\Phi]}{\delta\Phi_a(q)\delta\Phi_b(q')}\right|_{\Phi=\Phi_0} = (2\pi)^D\delta^{(D)}(q-q')\left(m^2+\lambda-q^2\right)\delta_{ab}, \end{aligned} \tag{17.100}$$

where the subscript c indicates the connected Green function. In mean-field theory, the first quantity behaved like

$$\langle \phi^2(x) \rangle = 0, \qquad \text{for } m^2 > 0, \quad (\tau > 0), \tag{17.101}$$

$$\langle \phi^2(x) \rangle = -\frac{Nm^2}{g} \sim -\frac{N\mu^2}{g}\tau, \qquad \text{for } m^2 < 0, \quad (\tau < 0). \tag{17.102}$$

The inverse susceptibility is for $T > T_c$

$$\chi(q) = m^2 + \mathbf{q}^2 - q_0^2 = \mu^2\tau + \mathbf{q}^2 - q_0^2, \tag{17.103}$$

and for $T < T_c$

$$\begin{aligned} \chi_{\|}(q) &= \mathbf{q}^2 - q_0^2, \\ \chi_{\perp}(q) &= -2m^2 + \mathbf{q}^2 - q_0^2 = -2\mu^2\tau + \mathbf{q}^2 - q_0^2. \end{aligned} \tag{17.104}$$

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[6] J. M. Kosterlitz and D. J. Thouless, J. Phys. C *6*, 1181 (1973); V. Ambegaokar and S. Teitel, Phys. Rev. B *19*, 1667 (1979).

These behaviors can be modified considerably by the radiative corrections calculated in the last section. Consider first the cases of one and two dimensions where there is no spontaneous symmetry breakdown. Here the susceptibility remains isotropic and finite for all temperatures. We calculate

$$\begin{aligned} \chi^{-1}(0) &= \lambda \\ \chi^{-1}(q) &= \lambda + \mathbf{q}^2 - q_0^2 \end{aligned} \qquad (17.105)$$

and see that far above T_c, χ^{-1} approaches the mean field value since there $\lambda \sim m^2 \sim \mu^2 T_c$. Close to T_c, however, $\chi_\perp^{-1}(0)$ goes no longer to zero. It smoothly becomes flatter and tends to zero like

$$\begin{aligned} \chi_\perp^{-1}(0) &\sim \mu^2 e^{\tau\mu^2 4\pi/g} && D=2 \\ \chi_\perp^{-1}(0) &\sim \frac{g^2}{4\mu^4}\tau^{-1} && D=1. \end{aligned}$$

This rapid falloff may be seen as a washed-out remnant of the original anisotropic vanishing of $\chi_\perp^{-1}(0)$ due to the Nambu-Goldstone modes. Here it is due to large *isotropic* pretransitional fluctuations. The expectations of $\langle\phi^2(x)\rangle$ can be obtained as follows: Differentiate the generating functional $Z[j]$ with respect to the mass square in the functional picture. Then we see that

$$2i\frac{\partial}{\partial m^2}Z[j] = \int \mathcal{D}\phi \left(\int d^D x \phi^2\right) e^{i\mathcal{A}[\phi]+i\int d^D x j(x)\phi(x)}. \qquad (17.106)$$

But this is, up to the normalization factor $Z[j]$, the Green function in the presence of the external field j:

$$\int d^D x \langle T\phi(x)\phi(x)\rangle_j. \qquad (17.107)$$

Explicitly

$$\int d^D x \langle\phi^2(x)\rangle j = Z^{-1}[j]\, 2i\frac{\partial}{\partial m^2}Z[j]. \qquad (17.108)$$

From this, the desired quantity $\langle\phi^2(x)\rangle$ can be calculated as

$$\langle 0|\phi^2(x)|0\rangle = \frac{1}{VT}Z^{-1}[0]2i\frac{\partial}{\partial m^2}Z[0]. \qquad (17.109)$$

Using the effective action this becomes

$$\langle 0|\phi^2(x)|0\rangle = -\frac{1}{VT}2\frac{\partial}{\partial m^2}\Gamma[\Phi] \qquad (17.110)$$

or with the effective potential

$$\langle 0|\phi^2(x)|0\rangle = 2\frac{\partial}{\partial m^2}v(\Phi). \qquad (17.111)$$

Inserting the previous results in one and two dimensions we find

$$\langle 0|\phi^2(x)|0\rangle = \frac{1}{g}\left(\lambda - m^2\right). \tag{17.112}$$

For large m, where $\lambda \to m^2$, this tends to zero, i.e., to the mean-field result. As m^2 goes to zero, however, the function remains smooth (and positive). As the temperature drops far below T_c $\left(m^2 \to -\infty\right)$, λ tends to zero and the behavior becomes again mean-field like.

We can summarize: In one- and two dimensional systems, the expectation value $\langle\phi^2(x)\rangle$ interpolates smoothly between the mean-field limits above and below T_c. The susceptibility $\xi^{-1}(0)$ does the same thing. Thereby it remains isotropic for all decreasing T.

Consider now the cases of 3 and 4-dimensions for which the only ground states with real potential $v(\Phi,\lambda)$ were found at $\lambda = 0$ and $\Phi_{0a} \neq 0$. In order to calculate the susceptibilities at $q = 0$ we write V in the form

$$v(\Phi,\lambda) = \frac{1}{2}\lambda\Phi_a^2 - \gamma(\lambda) \tag{17.113}$$

where

$$-2\gamma_4(\lambda) = -\frac{N}{2g}\lambda^2 + \frac{Nm^2}{g}\lambda + \frac{N}{4}S_4\lambda^2\left(\log\frac{\lambda}{\mu^2} - \frac{1}{2}\right)$$

and

$$-\,2\gamma_3(\lambda) = -\frac{N}{2g}\lambda^2 + \frac{Nm^2}{g}\lambda + N\frac{\pi}{3}S_3\lambda^{3/2} \tag{17.114}$$

in 4 and 3 dimensions, respectively. We have recorded the dimension as a subscript on $\gamma(\lambda)$. Let us now form the derivatives

$$V_{\Phi_a} = \lambda\Phi_a + \left[\frac{1}{2}\Phi_a^2 - \gamma_D'(\lambda)\right]\lambda_{\Phi_a}, \tag{17.115}$$

$$V_{\Phi_a\Phi_b} = \lambda\delta_{ab} + \left\{\left[\Phi_a\lambda_{\Phi_b} + (a \leftrightarrow b)\right] - \gamma''(\lambda)\lambda_{\Phi_a}\lambda_{\Phi_b}\right\} + \left[\frac{1}{2}\Phi_a^2 - \gamma(\lambda)\right]\lambda_{\Phi_a\Phi_b}. \tag{17.116}$$

We may now use the equation of state $\Phi^2 = 2\gamma'(\lambda)$ and its derivative $\Phi_a = \gamma''(\lambda)\lambda_{\Phi_a}$ to simplify (17.115) and write it as

$$V_{\Phi_a\Phi_b} = \lambda\delta_{ab} + \frac{\Phi_a\Phi_b}{\gamma''(\lambda)} = \lambda\left(\delta_{ab} - \frac{\Phi_a\Phi_b}{\Phi_c^2}\right) + \frac{\Phi_a\Phi_b}{\Phi_c^2}\left[\lambda + \frac{1}{\gamma''(\lambda)}\right]\Phi_c^2. \tag{17.117}$$

Thus we can identify the transverse susceptibility as

$$\xi_\perp^{-1}(0) = \lambda. \tag{17.118}$$

and the longitudinal one

$$\xi_{\parallel}^{-1}(0) \;=\; \left[\lambda+\frac{1}{1/\gamma''(\lambda)}\right]\Phi_c^2=2\left[\lambda+\frac{1}{\gamma''(\lambda)}\right]\gamma'(\lambda). \tag{17.119}$$

Actually, we could have obtained the result (17.116) from our earlier equations (17.48) where the full inverse Green function was derived. Inserting there

$$m_0^2+\Sigma=\lambda, \qquad \gamma(\Sigma)\to\gamma(\lambda), \tag{17.120}$$

we immediately verify (17.117).

For spontaneously broken symmetry, λ vanishes and we find

$$\xi_{\perp}^{-1}(0)=0 \tag{17.121}$$

just as in mean-field theory, since this is a rigorous consequence of the Nambu-Goldstone theorem. For the longitudinal component we obtain

$$\chi_{\parallel}^{-1}(0)=2\gamma'(0)/\gamma''(0). \tag{17.122}$$

Inserting (17.114) we have in 3 and 4 dimensions

$$\chi_{\parallel}^{-1}(0)=0. \tag{17.123}$$

This, contrary to the mean field case where $\xi_{\parallel}^{-1}(0)=-2m^2>0$, the longitudinal susceptibility diverges. At first sight we might be led to conclude that also the mode in the longitudinal direction has become massless due to fluctuations. It will turn out soon that this conclusion would be false. The nature of this singularity will be studied in more detail in the next section (Hugenholtz-Pines Theorem).

17.6 Correlation Functions for Large N

We have argued in Chapter 12 that the set of all vertex functions can be obtained from a finite number of tree diagrams which follow from the effective action $\Gamma[\Phi_0+\Phi',\Sigma_0+\Sigma']$ considered as a functional of Φ',Σ' [see the equations after (6.194)]. Let us therefore set

$$\lambda_0=m_0^2+\Sigma_0. \tag{17.124}$$

Inserting into the action (17.61) $\Sigma=\Sigma_0+\Sigma'$, we expand

$$\begin{aligned}\Gamma\left[\Phi,\Sigma_0+\Sigma'\right] \;=\;& \frac{1}{2}(\partial\Phi)^2-\frac{1}{2}\lambda_0\Phi^2-\frac{1}{2}\Sigma'\Phi^2+\frac{i}{2}N\mathrm{Tr}\log\left(-\partial^2-\lambda_0-\Sigma'\right)\\ &+\frac{N}{4g_0}\int d^Dx\Sigma'^2+\frac{N}{2g_0}\left(\lambda_0-m_0^2\right)\int d^Dx\Sigma'+\frac{N}{4g_0}\left(\lambda_0-m_0^2\right)^2.\end{aligned} \tag{17.125}$$

The value of Σ_0 or M_0 is determined by solving

$$\Gamma_{\Sigma'}\left[\Phi_{0a},\Sigma_0\right]=0 \tag{17.126}$$

This eliminates all graphs with a Σ' line ending in the vacuum (tadpole graphs). The same rules hold for $m^2 < 0$ in one and two dimensions where there is no spontaneous symmetry beakdown.

Consider now the non-trivial cases of $m^2 < 0$ in three and four dimensions. Again we can remove the Σ' tadpoles by going to the extremum. Contrary to (17.126), this lies now at

$$\Sigma_0 = \lambda_0 = 0 \tag{17.127}$$

with a non-zero value of Φ given by

$$\Phi_a^2 = \gamma'(0) = -\frac{N}{g_0} m_0^2. \tag{17.128}$$

Thus we may write the effective action as

$$\begin{aligned} \Gamma\left[\Phi, \Sigma_0 + \Sigma'\right] &= \frac{1}{2}\left(\partial\Phi_a\right)^2 - \frac{1}{2}\Sigma'\left[\Phi_a^2 - (\Phi_{0a})^2\right] \\ &+\frac{1}{2}\Sigma'\Gamma^{(2)}\Sigma' - i\frac{N}{2}\mathrm{Tr}\sum_{n=3}^{\infty}\left(-\frac{i}{-\partial^2}\Sigma'\right)^n\frac{1}{n} + \frac{N}{4g}m_0^4 \end{aligned} \tag{17.129}$$

This action is free of linear terms in Σ' if instead of the fields Φ_a one uses the shifted fields $\Phi_a' = \Phi_a - \Phi_{0a}$. The components of Φ_a parallel to Φ_{0a} call them $\Phi_{\|}$, In order to find the eigenmodes we have to diagonalize the matrix, written for euclidean momenta,

$$\begin{pmatrix} q^2 & \Phi_0 \\ \Phi_0 & \Gamma^{(2)}(q) \end{pmatrix} \tag{17.130}$$

where $\Phi_0 \equiv \sqrt{\Phi_{0a}^2}$. Let us write down $\Gamma^{(2)}$ explicitly as

$$\Gamma^{(2)}(q) = -\frac{1}{2}N\left[\frac{1}{g} + I(q)\right] \tag{17.131}$$

with

$$I(q) = \int\frac{d^Dk}{(2\pi)^D}\frac{1}{k^2(k+q)^2}. \tag{17.132}$$

In D dimensions, this was calculated in (5.135):

$$I(q) = S_D\frac{1}{2}\Gamma\left(2-\epsilon/2\right)\Gamma(\epsilon/2)\mu^{-\epsilon}\int_0^1 d^Dx\frac{\mu^\epsilon}{\left[q^2x(1-x)\right]^{\epsilon/2}}. \tag{17.133}$$

Consider first the case of 3 dimensions. Then $S_3 = 1/2\pi^2$ and the integral is finite

$$I(q) = \frac{1}{8\pi}\frac{\mu}{(q^2)^{1/2}}\int_0^1 d^Dx\left[x(1-x)\right]^{-1/2} = \frac{1}{8\sqrt{q^2}}. \tag{17.134}$$

Using this we find for the diagonalized modes

$$
\begin{aligned}
G_{\Phi'_{\|d}\Phi'_{\|d}} &= \frac{q+g/8}{q\left(q^2+qg/8-2m_2\right)} && (17.135)\\
G_{\Sigma'_d\Sigma'_d} &= \frac{gq^2}{N\left(m^2-qg/16-q^2/2\right)}. && (17.136)
\end{aligned}
$$

In the limit $g \to 0$, the first mode becomes the mean-field longitudinal particle of mass $-2m^2$ with the second mode disappearing.

We are now in a position to understand the divergence of the longitudinal susceptibility for $q^2 \to 0$. From (17.135) we see that the propagator has a square root singularity in q^2 at this point. This does not correspond to another zero-mass particle. It is generated by the possibility of the $\Phi_{\|d}$ particle to decay into two massless Nambu-Goldstone bosons if fluctuations are taken into account. As a matter of fact, the Φ_d mode does not have any proper particle nature: If we return from euclidean to physical values of q, the mean field pole at $q^2 = -2m^2$, is no longer visible but hides in the second sheet of a complex q^2 plane. This is cut from $q^2 = 0$ to $q^2 = \infty$. The physical region lies right above the cut, in accordance with the usual $-i\epsilon$ prescription for singularities (actually, due to the $-i\epsilon$ prescription, the cut has to be displaced slightly down by $i\epsilon$). The pole can only be reached one by passing the cut from above into the second sheet at

$$\sqrt{-q^2} = -\frac{g}{16} - \sqrt{2m^2 + \left(\frac{g}{16}\right)^2} \qquad (17.137)$$

i.e.,

$$q^2 = -2m^2 - 2\left(\frac{g}{16}\right)^2 - i\frac{g}{8}\sqrt{-2m^2 - \left(\frac{g}{16}\right)^2}.$$

There is another pole at the complex conjugate position above the axis but this is far away from the physical region above the cut: It can only be reached by circulating anticlockwise around the branch point and going into the second sheet from below.

Let us now look at the four-dimensional situation. Here $I(q)$ becomes with $S_4 = 1/8\pi^2$ [see (9.173) and (9.169)]

$$I(q) = \frac{1}{8\pi^2}\left(\frac{1}{\epsilon} + \frac{1}{2} - \frac{1}{2} + \log\frac{q^2}{\mu^2}\right). \qquad (17.138)$$

The $1/\epsilon$-singularity is absorbed in a renormalization of $1/g_0$ as in (17.71), and we have

$$\Gamma^{(2)}(q) = -\frac{N}{2}\left[\frac{1}{g} + \frac{1}{16\pi^2}\left(1 - \log\frac{q^2}{\mu^2}\right)\right] \qquad (17.139)$$

such that the diagonalized propagators become

$$G_{\Phi'_{\|d}\Phi'_{\|d}} = \frac{1}{2}\,\frac{1/g+\left(1-\log q^2/\mu^2\right)/16\pi^2}{-m^2/g+(q^2/2)\left[1/g+\left(1-q^2/\mu^2\right)/16\pi^2\right]} \tag{17.140}$$

$$G_{\Sigma'_d\Sigma'_d} = -\frac{1}{N}\frac{q^2}{-m^2/g+(q^2/2)\left[1/g+\left(1-q^2/\mu^2\right)/16\pi^2\right]} \tag{17.141}$$

Again we observe the cut in the q^2-plane, starting at $q^2=0$, which is now logarithmic rather than of the square root type due to the increased dimensionality of space time. In addition there is a conjugate pair of poles one near $+2m^2$ but hidden in the second sheet [see Fig. 8.1]. There is, however, an important difference with respect to the previous case. There is another pole in both propagators which cannot correspond to a physical particle since it lies at a large positive value of q^2 which corresponds to a particle moving with a velocity faster than light.

18

Non-Linear σ-Model

Another model which is exactly solvable in a limit $N \to \infty$ and illustrates some typical properties of quantum field theories is the so-called *non-linear σ-model.* It has its origin in statstical mechanics where it arises as a limit of the classical Heisenberg spin model of ferromagnetism. There ist is known under the name of *spherical model.* The nonlinear σ-model yields a complementary approach to the critical phenomena described previously by the O(N)-symmetric ϕ^4-theory.

18.1 Definition of Classical Heisenberg Model

The model consists of a fluctuating field $n_a(\mathbf{x})$ of unit vectors with N components

$$n_a(\mathbf{x}) \quad (a = 1, \dots, N), \qquad n_a^2(\mathbf{x}) = 1. \tag{18.1}$$

We shall discuss here the euclidean formulation in which the model is described by a partition function

$$Z = \prod_{\mathbf{x}} \left[\int \frac{d^{N-1} n_a(\mathbf{x})}{S_N} \right] \exp \left[-\frac{1}{2g} \int d^D x [\boldsymbol{\nabla} n_a(\mathbf{x})]^2 \right]. \tag{18.2}$$

The constant S_N is the surface of a sphere in N dimensions covered by the directional integral $d^D n^a$. This ensures a unit integral $\int d^{N-1} n^a / S_N = 1$. Explicitly, $S_N = 2\pi^{N/2}/\Gamma(N/2)$ [recall (9.125)]. This model can be thought of as arising from the euclidean action of a previous O(N)-symmetric ϕ^4-theory in Chapter 17,

$$\mathcal{A} = \int d^D x \left[\frac{1}{2} (\boldsymbol{\nabla} \phi_a)^2 + \frac{m^2}{2} \phi_a^2 + \frac{g}{4} \left(\phi_a^2 \right)^2 \right] \tag{18.3}$$

by going to the limit of very large negative m^2. For negative m^2, the O(N)-symmetry is spontaneously broken, and the N initially degenerate fluctuation modes decompose into a massive fluctuation of the size $\phi \equiv \sqrt{\phi_a^2}$ of the field (*radial fluctuations* in field space) and $N-1$ fluctuation modes of the direction of the field ϕ_a (*azimuthal fluctuations* in field space) described by the unit vectors

$$n_a \equiv \phi_a / \sqrt{\phi_a^2}. \tag{18.4}$$

These are the Goldstone bosons arising whenever there is a spontaneous breakdown of a continuous symmetry (see Section 15.2). In the limit $m^2 \to \infty$, the size fluctuations are completely frozen out. The action can be written approximately as

$$\mathcal{A} \xrightarrow[m^2\to-\infty]{} \int d^Dx \left[-\frac{(-m^2)^2}{4g} + \frac{1}{2}|\phi|^2(\boldsymbol{\nabla} n_a)^2 \right]. \tag{18.5}$$

Dropping the first term with the constant condensation energy, we arrive at the O(N) non-linear σ model (18.3) with a coupling constant

$$g = \frac{1}{|\phi|^2}. \tag{18.6}$$

Readers familiar with models of statistical mechanics will recognize the intimate relation of the model (18.2) with the so-called classical O(N)-symmetric *Heisenberg model of ferromagnetism*. It is defined on a lattice, where its energy is written as a sum over nearest-neighbor interactions between local D-dimensional spin vectors $\mathbf{S}_i$, which are conventionally normalized to unit length:

$$E = -\frac{J}{2} \sum_{\{i,j\}} \mathbf{S}_i \cdot \mathbf{S}_j \quad \text{with } J > 0 \text{ and } \mathbf{S}_i^2 = 1. \tag{18.7}$$

If $\mathbf{S}_i$ were not normali The index pairs i,j run over all nearest neighbor pairs. The spin vectors $\mathbf{S}_i$ fluctuate and represent the order field. The expectation value $\mathbf{M} \equiv \langle \mathbf{S}_i \rangle$ is called the magnetization. If $\mathbf{M}$ is nonzero, the system is said to exhibit a spontaneous magnetization. This happens only at low temperatures. Above a critical temperature $T_c^{\rm MF}$, the system is normal with $\mathbf{M} = 0$.

A special case of this model is the famous *Ising model* where the direction of the vector $\mathbf{S}_i$ is restricted to a single axis, pointing parallel or antiparallel to it. The phase transition of magnetic systems with strong anisotropy can be described by this model. Then $\mathbf{S}_i$ can be replaced by a scalar field with positive and negative signs, and the symmetry which is spontaneously broken in the low-temperature phase is the reflection symmetry $S(\mathrm{x}) \to -S(\mathrm{x})$.

Let us denote the lattice points by a vector $\mathbf{x}$ on a simple cubic lattice, i.e., we let $\mathbf{x}$ take the values

$$\mathbf{x}_{(m_1,m_1,\dots,m_d)} \equiv \Sigma_{i=1}^D m_i\, \mathbf{i}, \tag{18.8}$$

where $\mathbf{i}$ are the basis vectors of a D-dimensional hypercubic lattice, and m_i are integer numbers 0, ±1, ±2, … .

The partition function associated with the generalized Heisenberg model is

$$Z = \sum_{\substack{\text{spin}\\ \text{configurations}}} e^{-E/k_BT}, \tag{18.9}$$

where the sum runs over all possible spin configurations. The unit spin vectors $\mathbf{S}_i$ are now identified with the unit vector fields $\mathbf{n}(\mathbf{x})$ in (18.1). The sum over products $\Sigma_{\{i,j\}}\, \mathbf{n}_i \mathbf{n}_j$ in the energy (18.7) can then be rewritten as

$$\sum_{\{i,j\}} \mathbf{n}_i \mathbf{n}_j \;=\; \sum_{\{i,j\}} \Big[\mathbf{n}_i(\mathbf{n}_j - \mathbf{n}_i) + 1\Big] = 2\sum_{\mathbf{x}}\sum_{\mathbf{i}} \{\mathbf{n}(\mathbf{x})[\mathbf{n}(\mathbf{x}+\mathbf{i}) - \mathbf{n}(\mathbf{x})]) + 1\}$$

$$= -\sum_{\mathbf{x}}\left\{\sum_{\mathbf{i}}[\mathbf{n}(\mathbf{x}+\mathbf{i})-\mathbf{n}(\mathbf{x})]^2-2D\right\} \tag{18.10}$$

Now we introduce lattice gradients

$$\nabla_{\mathbf{i}}\,\mathbf{n}(\mathbf{x}) \equiv \frac{1}{a}\left[\mathbf{n}(\mathbf{x}+\mathbf{i})-\mathbf{n}(\mathbf{x})\right], \tag{18.11}$$

$$\overline{\nabla}_{\mathbf{i}}\,\mathbf{n}(\mathbf{x}) \equiv \frac{1}{a}\left[\mathbf{n}(\mathbf{x})-\mathbf{n}(\mathbf{x}-\mathbf{i})\right], \tag{18.12}$$

where a is the lattice spacing, and rewrite (18.10) as

$$\sum_{\{i,j\}}\mathbf{n}_i\mathbf{n}_j = -\sum_{\mathbf{x}}\left\{a^2\sum_{\mathbf{i}}[\nabla_{\mathbf{i}}\,\mathbf{n}(\mathbf{x})]^2-2D\right\}. \tag{18.13}$$

With this, the partition function (18.9) takes the form

$$Z=\prod_{\mathbf{x}}\left[\int\mathbf{n}(\mathbf{x})\right]\exp\left[-\frac{J}{2k_BT}\sum_{\mathbf{x}}\left(\sum_{\mathbf{i}}a^2[\nabla_{\mathbf{i}}\,\mathbf{n}(\mathbf{x})]^2-2D\right)\right]. \tag{18.14}$$

We can use the lattice version of partial integration[1]

$$\sum_{\mathbf{x}}\sum_{\mathbf{i}}[\nabla_{\mathbf{i}}\,f(\mathbf{x})]\,g(\mathbf{x})=-\sum_{\mathbf{x}}\sum_{\mathbf{i}}f(\mathbf{x})\overline{\nabla}_{\mathbf{i}}\,g(\mathbf{x}), \tag{18.15}$$

which is valid for all lattice functions with periodic boundary conditions, to express (18.13) in terms of a lattice version of the Laplace operator $\overline{\nabla}_{\mathbf{i}}\nabla_{\mathbf{i}}$, where repeated lattice unit vectors are summed. Then

$$\sum_{\mathbf{x}}\left\{\sum_{\mathbf{i}}a^2[\nabla_{\mathbf{i}}\,\mathbf{n}(\mathbf{x})]^2-2D\right\}=-\sum_{\mathbf{x}}\left[a^2\,\mathbf{n}(\mathbf{x})\overline{\nabla}_{\mathbf{i}}\nabla_{\mathbf{i}}\,\mathbf{n}(\mathbf{x})+2D\right]. \tag{18.16}$$

Ignoring the irrelevant constant term $\Sigma_{\mathbf{x}}2D$, we can then write the sum over all spin configurations in the partition function (18.9) as a product of integrals over a unit sphere at each lattice point

$$Z=\prod_{\mathbf{x}}\left[\int\mathbf{n}(\mathbf{x})\right]\exp\left\{\frac{Ja^2}{2k_BT}\sum_{\mathbf{x}}\mathbf{n}(\mathbf{x})\overline{\nabla}_{\mathbf{i}}\nabla_{\mathbf{i}}\,\mathbf{n}(\mathbf{x})\right\}. \tag{18.17}$$

For small a, the sums (18.16) have continuum limit

$$a^{2-D}\int d^Dx\left\{[\boldsymbol{\nabla}n_a(\mathbf{x})]^2-\frac{2D}{a^2}\right\}=-a^{2-D}\int d^Dx\left\{n_a(\mathbf{x})\boldsymbol{\nabla}^2n_a(\mathbf{x})+\frac{2D}{a^2}\right\}. \tag{18.18}$$

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[1] For the handling of lattice gradients see Section 2.2 in the textbook H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics,* World Scientific Publishing Co., Singapore 1995.

After dropping the irrelevant D/a^2 term, the Boltzmann factor in the partition function (18.17) agrees with the exponential in the partition function (18.2) of the non-linear σ-model with a coupling constant

$$g = \frac{k_B T}{J} a^{D-2}. \tag{18.19}$$

In these models, g grows with the temperature, and because of the significance of the model for statistical mechanics we shall find it convenient to replace the prefactor $1/g$ in (18.2) by a reduced inverse temperature $1/T$, discussing the model as a function of the reduced temperature rather than coupling strength. As we see from (18.19), this reduced temperature corresponds to the true one if the true one is measured in units of J/a^{D-2}.

As mentioned in the beginning of this chapter, the limit $N \to \infty$ of this model is referred to as the *spherical model.*

18.2 Spherical Model

The $N \to \infty$ -limit of the Heisenberg model was first solved by Berlin and Kac in 1952.[2] The solution of the model is quite simply. We liberate n_a from its constraint $n_a^2 = 1$, allowing each component to fluctuate between $-\infty$ and ∞. The constraint is enforced by an extra functional integral over a Lagrange multiplier $\lambda(\mathbf{x})$. Thus we write the lattice partition function as

$$Z = \prod_{\mathbf{x}} \left[\int_{-i\infty}^{i\infty} \frac{d\lambda(\mathbf{x})}{4\pi i T} \int_{-\infty}^{\infty} \frac{d^N n_a(\mathbf{x})}{S_N} \right] \exp\left\{ -\frac{1}{2g} \int d^D x \left[(\boldsymbol{\nabla} n_a)^2 + \lambda \left(n_a^2 - 1 \right) \right] \right\}. \tag{18.20}$$

In this form, the integrals over the components n_a are Gaussian, so that they can be done, leaving a functional integral over only $\lambda(\mathbf{x})$:

$$Z = \prod_{\mathbf{x}} \left[\int_{-i\infty}^{i\infty} \frac{d\lambda(\mathbf{x})}{4\pi i T} \right] \exp\left[-\frac{N}{2} \mathrm{Tr} \log\left[-\boldsymbol{\nabla}^2 + \lambda(\mathbf{x}) \right] + \frac{1}{2T} \int d^D x \lambda(\mathbf{x}) \right]. \tag{18.21}$$

In the limit $N \to \infty$, this is the partition function of the spherical model. In this limit, the first term in the exponent grows so large that the λ fluctuations become frozen at the extremum of the action. The limit is non-trivial if we allow g^{-1} to carry a factor N. Thus we set

$$g \equiv t/N. \tag{18.22}$$

Now we can go to large N, and find a partition function

$$Z \xrightarrow[N \to \infty]{} e^{-F/t}, \tag{18.23}$$

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[2] T.H. Berlin and M. Kac, Phys. Rev. *86*, 82 (1952).

with the free energy per O(N)-degree of freedom and per temperature unit

$$\frac{F}{t} \xrightarrow[N\to\infty]{} \frac{1}{2}\left[\mathrm{Tr}\,\log\left[-\boldsymbol{\nabla}^2+\lambda(\mathbf{x})\right]-\frac{1}{t}\int d^Dx\lambda(\mathbf{x})\right], \tag{18.24}$$

to be evaluated at the extremum where the functional derivative $\delta F/\delta\lambda(\mathbf{x})$ vanishes. Explicitly, this condition reads

$$\frac{1}{t}=[-\boldsymbol{\nabla}^2+\lambda(\mathbf{x})]^{-1}(\mathbf{x},\mathbf{x}). \tag{18.25}$$

Each solution $\lambda_i(\mathbf{x})$ of this equation must be found, and the partition function is given by the sum over the Boltzmann factors (18.23) for all of them. In general, these solutions are hard to find. One solution, however, is straightforward: that with a constant $\lambda(\mathbf{x})\equiv\lambda$, for which the free energy (18.26) becomes

$$\frac{F}{tL^D} \xrightarrow[N\to\infty]{} \frac{1}{2}\left[\int\frac{d^Dp}{(2\pi)^D}\log\left(\mathbf{p}^2+\lambda\right)-\frac{1}{t}\int d^Dx\lambda\right], \tag{18.26}$$

where L^D is the spatial volume of the system, and the extremality condition (18.25) turns into the so-called *gap equation*:

$$\frac{1}{t}=\int\frac{d^Dk}{(2\pi)^D}\frac{1}{k^2+\lambda}. \tag{18.27}$$

This solution will now be discussed.

18.3 Free Energy and Gap Equation in $D > 2$ Dimensions

Using formulas (9.133) and (9.135), the integrals in (18.26) and (18.27) can be done right-away in D dimensions with the result

$$\frac{F}{tL^D} \;\xrightarrow[N\to\infty]{}\; \frac{1}{2}\bar{S}_D\frac{1}{D}\Gamma\left(\frac{D}{2}\right)\Gamma\left(1-\frac{D}{2}\right)\lambda^{D/2}-\frac{\lambda}{2t} \tag{18.28}$$

for the free energy and

$$\frac{1}{t} \;=\; \bar{S}_D\frac{1}{2}\Gamma\left(\frac{D}{2}\right)\Gamma\left(1-\frac{D}{2}\right)\lambda^{D/2-1} \tag{18.29}$$

for the gap equation, where $\bar{S}_D=S_D/(2\pi)^D=2/(4\pi)^{D/2}\Gamma(D/2)$ from Eq. (9.128). It is easy to check that the free energy (18.28) is extremal for λ satisfying (18.29).

In order to discuss the physical consequences of these equations, consider first the case of two dimensions. Letting $\epsilon\equiv D-2$ approach zero, the equations become

$$\frac{F}{tL^D} \;\xrightarrow[N\to\infty]{}\; -\frac{1}{2}\bar{S}_D\frac{1}{\epsilon}\frac{1}{1+\epsilon/2}\lambda^{1+\epsilon/2}-\frac{\lambda}{2t}+\mathcal{O}(\epsilon), \tag{18.30}$$

$$\frac{1}{t} \;=\; -\bar{S}_D\frac{1}{\epsilon}\lambda^{\epsilon/2}+\mathcal{O}(\epsilon). \tag{18.31}$$

Note that we use ϵ for the deviations from $D = 2$ dimensions, in contrast to ε for th deviations from $D = 4$.

The gap equation has a solution. only for *negative* t. To avoid the infinities in the limit $\epsilon \longrightarrow 0$, we introduce an arbitrary mass scale μ and a renormalized temperature t_R via the defining equation for t_R:

$$\frac{1}{t} \equiv \frac{\mu^\epsilon}{t_R} - \bar{S}_D \frac{1}{\epsilon} \mu^\epsilon \tag{18.32}$$

Then we can take the limit $\epsilon \longrightarrow 0$ and find

$$\frac{F}{tL^D} \xrightarrow[N\to\infty]{} -\bar{S}_D \frac{1}{4} \lambda \left(\log \frac{\lambda}{\mu^2} - 1 \right) - \frac{\lambda}{2t_R} \tag{18.33}$$

$$\frac{1}{t_R} = -\bar{S}_D \frac{1}{2} \log \frac{\lambda}{\mu^2}. \tag{18.34}$$

The renormalized gap equation is solved for $\lambda = \bar{\lambda}$ satisfying the equation

$$\frac{\bar{\lambda}}{\mu^2} = e^{-2/t_R \bar{S}_D}. \tag{18.35}$$

For this value, the free energy has a maximum (see Fig. 18.1). This corresonds to a minimum in the λ-integrals in (18.21) which runs along the imaginary direction. Only the immediate neighborhood of this minimum contributes to the integral.

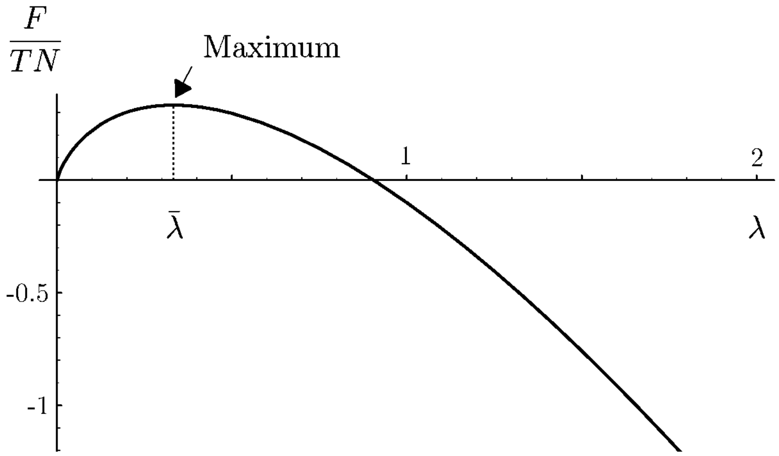

FIGURE 18.1 Free energy as a function of λ for $D = 2$ (schematically). The gap equation determines the position $\bar{\lambda}$ of the maximum.

The value of λ at the minimum is a parameter characterizing the solution, having the dimension of a square mass. From the role which λ plays in Eq. (18.20) and in the trace of the logarithm of the fluctuations (18.21) we see that λ is the square mass of the n_a-fluctuations. This implies that even though we had started out with a model describing $N - 1$ massless Goldstone bosons, the interacting system is not massless but all N fields have acquired a nonzero mass $M = \sqrt{\lambda}$. What we witness here is the *spontaneous restoration* of the O(N)-symmetry due to the violence of the directional fluctuations in two dimensions.

It is instructive to consider also the case of more than two dimensions and treat it in a way which has a smooth limit for $\epsilon \equiv D - 2 \to 0$. If ϵ is arbitrary, the free energy in $D \equiv 2 + \epsilon$ dimensions becomes

$$\frac{F(\lambda)}{tL^D} = -\frac{c_\epsilon}{2} \frac{\lambda^{1+\epsilon/2}}{1+\epsilon/2} - \frac{\lambda}{2t}, \tag{18.36}$$

where

$$c_\epsilon \equiv -\frac{S_D}{2} \Gamma\left(\frac{D}{2}\right) \Gamma\left(1 - \frac{D}{2}\right) = \frac{1}{\epsilon} S_D \frac{\pi\epsilon/2}{\sin(\pi\epsilon/2)}. \tag{18.37}$$

For small ϵ this behaves like

$$c_\epsilon \approx \frac{1}{2\pi\epsilon} + \mathcal{O}(\epsilon). \tag{18.38}$$

To have a smooth limit $\epsilon \to 0$ -limit of the free energy, we write

$$\frac{F(\lambda)}{tL^D} = \left\{ -\frac{1}{2} \frac{c_\epsilon}{1+\epsilon/2} \left[\left(\frac{\lambda}{\mu^2} \right)^{\epsilon/2} - \left(1 + \frac{\epsilon}{2} \right) \right] \lambda - \frac{\lambda}{2t_R} \right\} \mu^\epsilon \tag{18.39}$$

where t_R is the renormalized temperature defined by

$$\frac{1}{t} \equiv \frac{\mu^\epsilon}{t_R} - c_\epsilon \mu^\epsilon. \tag{18.40}$$

18.3.1 High-Temperature Phase

At high temperatures, where t_R is large, the free energy (18.36) has a maximum, as can be seen in Fig. 18.2. The position $\lambda = \bar{\lambda}$ of the maximum is determined by the unrenormalized gap equation as

$$\frac{1}{t} = -c_\epsilon \bar{\lambda}^{\epsilon/2} \tag{18.41}$$

For $2 > \epsilon > 0$, i.e., between two and four dimensions, there is a solution for the bare parameter $t < 0$. Equation (18.40) implies that in this regime the renormalization temperature is larger than a certain critical value t_R^c given by

$$t_R^c = c_\epsilon^{-1} > 0. \tag{18.42}$$

In terms of t_R, Eq. (18.40) reads

$$\frac{1}{t} = \mu^\epsilon \left(\frac{1}{t_R} - \frac{1}{t_R^c} \right), \tag{18.43}$$

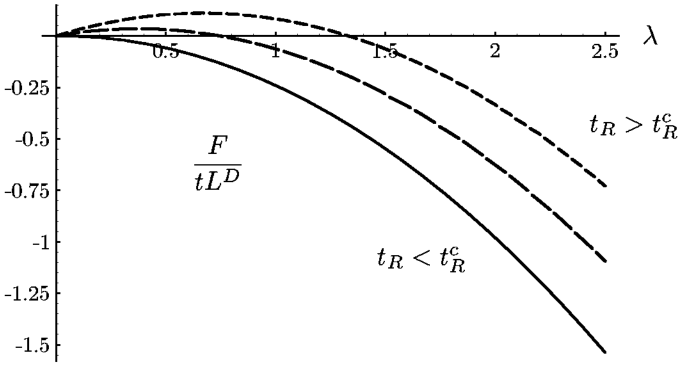

FIGURE 18.2 Free energy as a function of λ for $D = 2$ (schematically). The gap equation determines the position $\bar{\lambda}$ of the maximum.

and Eq. (18.43) gives the gap $\bar{\lambda}$ as a function of $t_R > t_R^c$:

$$\bar{\lambda} = \mu^2 \left(1 - \frac{t_R^c}{t_R}\right)^{2/\epsilon}. \tag{18.44}$$

For $t_R < t_R^c$, the maximum lies at $\lambda = \bar{\lambda} = 0$, as can be seen in Fig. 18.2.

Note that in order to make the functional integral of the theory (18.20) well-defined for $t_R > t_R^c$ where $t < 0$, the n^a-integrations have to be taken along the imaginary field axis. We shall see later in Section 18.5 that this apparently unphysical condition is an artifact of the analytic continuation in the dimension D.

18.3.2 Low-Temperature Phase

In the low-temperature regime

$$t_R < t_R^c, \tag{18.45}$$

where the unrenormalized temperature is positive, the gap equation (18.41) has no solution. The reason for this is an incorrect treatment of the fluctuations at zero momentum. In order to see what went wrong in the above calculations we may proceed in two ways. One is inspired by the treatment in Subsection 2.14.3 of the ideal Bose gas at a fixed particle number N. There we observed that the equation for the particle number containing a momentum integral over the Bose distribution could be performed only down to a certain temperature, where the chemical potential first hits zero (from the negative side). For low temperatures, the state of zero momentum accumulates a macroscopic number of states, the so-called *condensate*. To account for its presence, it was essential to treat the system in a finite volume, where the momenta have to be summed rather than being integrated over. Then, the zero-momentum state can be isolated and treated separately. This is a typical solution of an infrared problem of a field system. Let us do the same thing here.

If the system is enclosed in a box of volume L^D, we calculate the free energy (18.24) as

$$\frac{F}{tL^D} = \frac{1}{2L^D}\log\lambda + \frac{1}{2L^D}\sum_{\mathbf{k}\neq 0}\log\left(\mathbf{k}^2+\lambda\right) - \frac{\lambda}{2t}. \tag{18.46}$$

The first term is responsible for generating a local maximum at a real $\lambda = \bar\lambda$ which is a minimum for the $\delta\lambda$-fluctuations along the imaginary axis. The maximum lies at

$$\frac{1}{L^D}\frac{1}{\bar\lambda} + \frac{1}{L^D}\sum_{\mathbf{k}\neq 0}\frac{1}{\mathbf{k}^2+\bar\lambda} = \frac{1}{t}. \tag{18.47}$$

If the system has more than two dimensions, the sum over $1/(\mathbf{k}^2+\lambda)$ with $\mathbf{k}\neq 0$ can be replaced by a phase space integral $\int d^Dk\, L^D/(2\pi)^D(\mathbf{k}^2+\lambda)$. The relative error is only of order $1/\lambda L^2$, which can be calculated exactly using a D-dimensional version of the Euler-Maclaurin approximationEuler-Maclaurin approximation to sum in Eq. (5.669). Thus the gap equation (18.41) reads, more precisely,

$$\frac{1}{t} = \frac{1}{L^D\bar\lambda} - c_\epsilon\bar\lambda^{\epsilon/2}. \tag{18.48}$$

For $t<0$, this equation has for large volume L^D the same solution $\bar\lambda$ as before in (18.41), since the first term $1/L^D\bar\lambda$ on the right-hand side can be ignored. For $t>0$, however, this term makes an essential difference. It gives rise to a nonzero solution $\bar\lambda$, which is vanishingly small in the limit of infinite volume L^D. Here the second term in (18.48) can be neglected with respect to the first term, so that for positive t:

$$\bar\lambda \approx \frac{t}{L^D}. \tag{18.49}$$

The general solution for both finite and infinite volumes L^D is illustrated in Fig. 18.3. In the limit of infinite volume, the solution is

$$\begin{aligned}\bar\lambda &= 0, \qquad t\geq 0,\\ \bar\lambda &> 0, \qquad t<0.\end{aligned} \tag{18.50}$$

There is a phase transition at $t=0$. For $t>0$, all modes become massive and the O(N) symmetry is restored. For $t<0$, the original $N-1$ massless Goldstone modes survive.

What does this imply for the renormalized quantities? Using (18.42) and (18.43), we find from (18.48) the properly renormalized gap equation correcting the previous Eq. (18.44):

$$1-\frac{t_R^c}{t_R} = -\frac{t_R^c}{\mu^\epsilon L^D\bar\lambda} + \left(\frac{\bar\lambda}{\mu^2}\right)^{\epsilon/2} \tag{18.51}$$

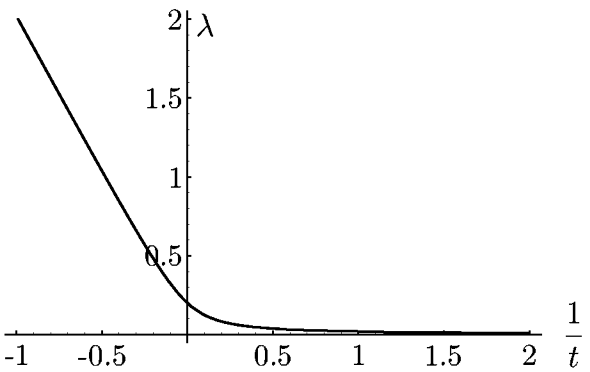

FIGURE 18.3 Solution of the gap equation (18.48) for $\epsilon = 1$ and large volume L^D. For $L \to \infty$, the right-hand part of the curve approaches more and more the abscissa.

For $t_R \geq t_R^c$ and large volume L^D, we can neglect the first term on the right-hand side, and (18.51) coincides with (18.44). For $t_R < t_R^c$, on the other hand, we can neglect the second term on the right-hand side, and find for the spontaneously generated square mass $\bar{\lambda}$ of the n_a-fluctuations:

$$\bar{\lambda} \approx \frac{t_R}{(\mu L)^\epsilon L^2}\left(1 - \frac{t_R}{t_R^c}\right)^{-1}. \tag{18.52}$$

This almost zero part of the gap in the low-temperature phase is pictured by the right-hand branch in Fig. 18.3. In the thermodynamic limit of infinite volume, $\bar{\lambda}$ goes to zero. In this limit, the system has a phase transition at the critical temperature $t_R^c > 0$, where the symmetry changes as described above. The statements for $t < 0$ and $t > 0$ hold now for $t_R > t_R^c$ and $t_R < t_R^c$, respectively. This is, of course, the same transition found earlier in the O(N)-symmetric ϕ^4-theory, only in quite a different description.

In a finite volume, the square mass $\bar{\lambda}$ is always nonzero, and there exists no phase in which the n_a-fluctuations are massless. The spontaneous breakdown of O(N)-symmetry is always restored by fluctuations.

18.4 Approaching the Critical Point

It is instructive to study the way in which the mass vanishes as t_R approaches t_R^c from above. From (18.44) we know that

$$\bar{\lambda} = \mu^2\left(1 - \frac{t_R^c}{t_R}\right)^{2/\epsilon}. \tag{18.53}$$

Since $\bar{\lambda}$ is the square mass of the n_a fluctuations, this implies that the correlation functions of the n^a fields fall of exponentially with

$$\langle n_a(\mathrm{x}) n_a(0)\rangle \xrightarrow[x\to\infty]{} e^{-|\mathrm{x}|/\xi} \tag{18.54}$$

where $\xi = \bar{\lambda}^{-\frac{1}{2}}$ is the correlation length. As t_R approaches the critical temperature, ξ goes to infinity according to the power law

$$\xi \sim (t_R - t_R^c)^{-\nu} \tag{18.55}$$

with

$$\nu = \frac{1}{\epsilon}. \tag{18.56}$$

This number is called the critical exponent of the correlation length. The power behavior of ξ as a function of temperature is shown in Fig. 18.4. A similar power behavior will be obtained later, in Chapter 21, for finite N as well, using renormalization group techniques, although for finite N it will no longer be possible to find an exact exact result.

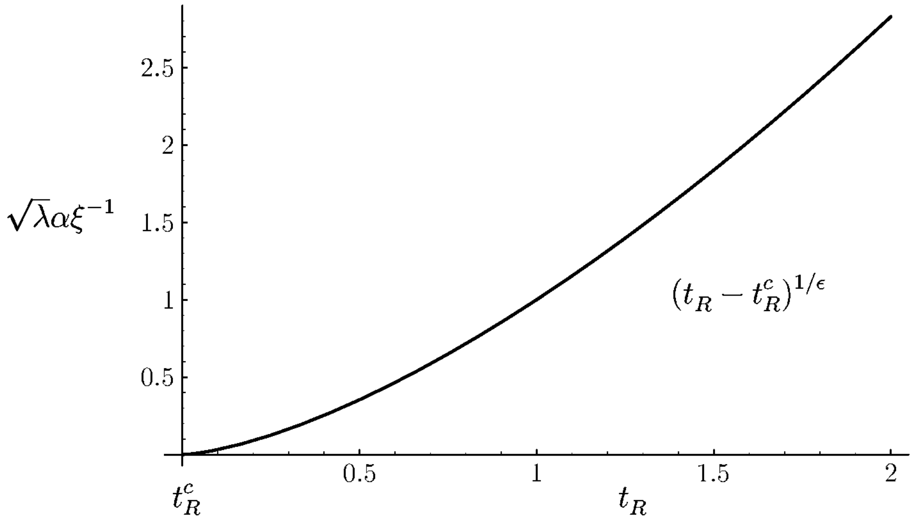

FIGURE 18.4 Temperature behavior of the correlation length.

18.5 Physical Property of Bare Temperature

The reader may rightfully wonder whether the entire treatment is consistent. We have observed above that the phase in which the symmetry has been restored possesses a negative bare temperature. This is not the sign of t which the model was originally defined with. Only for field integrations dn^a along the imaginary field direction does the partition function make sense. Fortunately, this apparent inconsistency is not intrinsic to the theory, but merely a mathematical artefact of the dimensional regularization of the divergent integral. A more physical regularization would have proceeded via a cutoff Λ in momentum space. Let us verify how this would change the range of the bare temperature where the phase transition takes place at a positive t.

In order to be specific, consider first the cases of $D=2$ and 3 dimensions. Using the integrals

$$\begin{aligned}\int_{|k|<\Lambda}\frac{d^2k}{(2\pi)^2}\log\left(k^2+\lambda\right) &= \frac{1}{4\pi}\left[\left(\Lambda^2+\lambda\right)\log\left(\Lambda^2+\lambda\right)-\Lambda^2-\lambda\log\lambda\right]\\ &\underset{\Lambda\to\infty}{\longrightarrow} \frac{1}{4\pi}\left[\Lambda^2\left(\log\Lambda^2-1\right)+\left(\log\Lambda^2+1\right)\lambda-\lambda\log\lambda\right],\end{aligned} \tag{18.57}$$

$$\begin{aligned}\int_{|k|<\Lambda}\frac{d^3k}{(2\pi)^3}\log\left(k^2+\lambda\right) &= \frac{1}{6\pi^2}\left\{\Lambda^3\log\left(\Lambda^2+\lambda\right)-\frac{2}{3}\Lambda^3+3\Lambda\lambda-2\lambda^{\frac{3}{2}}\arctan\frac{\Lambda}{\sqrt{\lambda}}\right\}\\ &\underset{\Lambda\to\infty}{\longrightarrow} \frac{1}{6\pi^2}\left[\Lambda^3\left(\log\Lambda^2-\frac{2}{3}\right)+3\Lambda\lambda-\pi\lambda^{\frac{3}{2}}\right],\end{aligned} \tag{18.58}$$

the free energy (18.24) becomes

$$\frac{F}{tL^2} = \frac{1}{2}\frac{1}{4\pi}\left[\Lambda^2\left(\log\Lambda^2-1\right)+\left(\log\Lambda^2+1\right)\lambda-\lambda\log\lambda\right]-\frac{\lambda}{2t}, \tag{18.59}$$

$$\frac{F}{tL^3} = \frac{1}{2}\frac{1}{6\pi^2}\left[\Lambda^3\left(\log\Lambda^2-\frac{2}{3}\right)+3\Lambda\lambda-\pi\lambda^{3/2}\right]-\frac{\lambda}{2t}. \tag{18.60}$$

In writing these expressions, we have assumed all momenta and masses to be dimensionless quantities. For proper expressions, all these quantities should be divided by some standard mass μ, which we set equal to one.

The dimensionally regularized expression (18.36), on the other hand, reads for dimensions $D=2+\epsilon$ with small $\epsilon>0$, and for $D=3$, respectively:

$$\frac{F}{tL^2N} = -\frac{1}{4}\frac{1}{2\pi}\frac{2}{\epsilon}\lambda-\frac{1}{4}\frac{\lambda}{2\pi}\log\frac{\lambda}{\mu^2}-\frac{\lambda}{2t}, \tag{18.61}$$

$$\frac{F}{tL^3N} = -\frac{1}{4}\frac{1}{2\pi}\frac{2}{3}\lambda^{\frac{3}{2}}-\frac{\lambda}{2t}. \tag{18.62}$$

For $D=2+\epsilon$, the positively divergent cutoff expression $\left(\log\Lambda^2+1\right)\lambda/8\pi$ in the second term of (18.60) is replaced by the negatively divergent $-\lambda/4\pi\epsilon$ in the first term of (18.61). For $D=3$, dimensional regularized expression in (18.62) shows no trace of the infinite linearly divergent term $\Lambda\lambda/4\pi^2$ in (18.60).

Thus the inverse temperature $1/t$ in the dimensionally regularized expressions must be thought of as being an unphysical version of the original inverse temperature $1/t$ in the initial bare energy, from which the constants $[\left(\log\Lambda^2+1\right)+2/\epsilon]/4\pi$ for $D=2$, or $\Lambda/2\pi^2$ for $D=3$, have been subtracted. Since these are very large quantities, there is no wonder that the dimensionally regularized discussion yields the phase with restored symmetry at a negative unphysical t.

The analytic continuation is taking advantage of the inobservability of the bare value of t in a continuous field theory. In any system in which there are well-defined physical mechanisms which regularize the short-wavelength fluctuations (for example lattice structures) and in which the bare temperature t is measurable by microscopic methods, the dimensional regularization cannot be used directly to properly represent the physical circumstances of the bare theory. This must be kept in mind when applying this method. This is, for example, the case in O(N)-lattice models of statistical mechanics to which the present non-linear σ-model is related via the continuum limit. This will be discussed in the next section.

18.6 Spherical Model on Lattice

In order to illustrate the point made in the last section it is instructive to go through the discussion once more in the lattice formulation of the spherical model. Then the lattice spacing a provides us with a natural short-distance cutoff, so that there is no need for introducing a momentum space cutoff Λ, nor dimensional regularization. On a simple hypercubic lattice, the partition function (18.17) reads

$$Z = \prod_{\mathbf{x}} \left[\int \frac{d\lambda(\mathbf{x})\beta a^2}{4\pi i} \right] \prod_{\mathbf{x}} \left[\int \frac{d^D n_a(\mathbf{x})}{S_D} \right] \exp\left(-\frac{\beta a^2}{2} \sum_{\mathbf{x}} \left\{ \left[(\nabla_i n)^2 + \lambda n^2 \right] - \lambda) \right\} \right), \tag{18.63}$$

where the gradient term has been brought to the lattice form (18.14) without the irrelevant term $-2D$. The dimensionless parameter

$$\beta \equiv \frac{1}{T} = \frac{J}{k_B T} \tag{18.64}$$

is called the *stiffness* of the directional fluctuations. The free energy per lattice site is given by

$$\beta f = \frac{1}{2} \left(\int_{-\pi/a}^{\pi/a} N \frac{d^D k a^D}{(2\pi)^D} \log \left\{ \sum_{i=1}^{D} [2 - 2\cos(k_i a)] + a^2 \lambda \right\} - \beta a^2 \lambda \right). \tag{18.65}$$

where $a^{-2} \sum_{i=1}^{D} [2 - 2\cos(k_i a)]$ is the Fourier transform of the lattice Laplacian $-\nabla_i \bar{\nabla}_i$. Extremizing this with respect to λ yields the gap equation

$$\beta = N v^D_{a^2\lambda}(\mathbf{0}), \tag{18.66}$$

where

$$v^D_{a^2 m^2}(\mathbf{x}) = \int_{-\pi/a}^{\pi/a} \frac{d^D k\, a^D}{(2\pi)^D} \frac{e^{i\mathbf{k}\mathbf{x}}}{\sum_{i=1}^{D} [2 - 2\cos(k_i a)] + a^2 m^2} \tag{18.67}$$

is the dimensionless lattice Green function of mass m in D dimensions. For small β, i.e., high temperatures, the gap equation has a solution $\lambda > 0$ and the fluctuations are massive. The solution exists up to a critical β_c given by

$$\beta_c = N v_0^D(\mathbf{0}). \tag{18.68}$$

For $D = 2$, the momentum integral diverges at the origin: $v_0^2(\mathbf{0}) = \infty$. This implies $\beta_c = 0$, so that a nonzero λ exists for all temperatures T larger than zero. Here the approximation (18.68) becomes useless, and a special discussion is necessary. This will be given in Subsection 19.2.5.

The Green function (18.67) is the dimensionless lattice version of the Yukawa potential in D dimensions

$$V_{m^2}^D(\mathbf{x}) = \int \frac{d^Dk}{(2\pi)^D} \frac{e^{i\mathbf{kx}}}{\mathbf{k}^2 + m^2}. \tag{18.69}$$

The lattice version has the Fourier representation

$$v_{a^2m^2}^D(\mathbf{x}) = \prod_i \left[\int_{-\pi/a}^{\pi/a} \frac{d(ak_i)}{2\pi}\right] \frac{e^{i\mathbf{kx}}}{\sum_{i=1}^D (2 - 2\cos ak_i) + a^2m^2}. \tag{18.70}$$

The denominator can be rewritten as $\int_0^\infty ds\, e^{-s\left[\sum_{i=1}^D (2-2\cos ak_i)+a^2m^2\right]}$, leading to the multiple integral

$$v_{a^2m^2}^D(\mathbf{0}) = \int_0^\infty dse^{-s(a^2m^2+2D)} \prod_{i=1}^D \left[\int_{-\pi}^{\pi} \frac{d\kappa_i}{2\pi} e^{2s\cos\kappa_i}\right]. \tag{18.71}$$

The integrations over k_i can now easily be performed, and we obtain the integral representation

$$v_{a^2m^2}^D(\mathbf{0}) = \int_0^\infty dse^{-s(a^2m^2+2D)} [I_0(2s)]^D, \tag{18.72}$$

where $I_0(2s)$ is the modified Bessel function. Integrating this numerically, we find for $D = 3, 4, \ldots, \ldots$ the values shown in Table 18.1.[3] A power series expansion of the Dth power of the modified Bessel function in (18.72),

$$[I_0(2s)]^D = 1 + Ds^2 + D(2D-1)\frac{s^4}{4} + D(6D^2 - 9D + 4)\frac{s^3}{36} + \ldots\ , \tag{18.73}$$

leads to the so-called *hopping expansion* for $v_{a^2\lambda}^D(\mathbf{0})$:

$$v_{a^2\lambda}^D(\mathbf{0}) = \frac{1}{2D + a^2\lambda} + \frac{2D}{(2D + a^2\lambda)^3} + \frac{6D(2D-1)}{(2D + a^2\lambda)^5} + \frac{20D(6D^2 - 9\ D + 4)}{(2D + a^2\lambda)^7} + \mathcal{O}(D^{-9}), \tag{18.74}$$

TABLE 18.1 Values of the lattice Yukawa potential $v_{l^2}^D(\mathbf{0})$ of reduced mass l^2 at the origin for different dimensions and l^2. The lower entries show the approximate values from the hopping expansion (18.74).

D	$v_0^D(\mathbf{0})$	$v_1^D(\mathbf{0})$	$v_2^D(\mathbf{0})$	$v_3^D(\mathbf{0})$	$v_4^D(\mathbf{0})$
3	0.2527	0.1710	0.1410	0.1214	0.1071
	0.2171	0.1691	0.1407	0.1214	0.1071
4	0.1549	0.1271	0.1105	0.0983	0.0888
	0.1496	0.1265	0.1104	0.0983	0.0888

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[3] See Tables on p.178 and p. 241 of the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I World Scientific, Singapore, 1989, and Eq. (6A.41) on p. 239.

which converges rapidly for large D, and yields for $D = 3, 4$ to the approximate values shown in the lower entries of Table 18.1. They lie quite close to the exact values in the upper part.

The lattice potential at the origin $v^D_{a^2\lambda}(\mathbf{0})$ in the gap equation (18.66) is always smaller than the massless potential $v^D_0(\mathbf{0})$. A nonzero value for λ can therefore only be found for sufficiently small values of the stiffness β, i.e., for sufficiently high temperatures T [recall (18.64)]. The temperature T_c at which the gap equation (18.66) has the solution $\lambda = 0$ determines the Curie point. Thus we have

$$T_c = \frac{J}{\beta_c k_B}, \tag{18.75}$$

where β_c is the critical stiffness (18.68):

$$\beta_c = N v^D_0(\mathbf{0}). \tag{18.76}$$

This result, derived for large N, turns out to be amazingly accurate even for rather small N. As an important example, take $N = 2$ where the model consists of planar spins and is referred to as XY-model. For $D = 3$, it describes accurately the critical behavior of the superfluid transition in helium near the λ-transition. From (18.76) and the value $v^D_0(\mathbf{0}) \approx 0.2527$ in Table 18.1 we estimate the critical value

$$\beta_c \approx 0.5054. \tag{18.77}$$

In Monte-Carlo simulation of this model one obtains, on the other hand,[4]

$$\beta_c \approx 0.45. \tag{18.78}$$

Thus, in three dimensions, we can us the large-N result (18.76) practically for all $N \geq 2$.

For $D > 2$, where β_c has a finite positive value, the solution for $\beta > \beta_c$ requires special consideration. The situation is similar to what we encountered earlier in the free Bose liquid. A condensate forms, consisting of Goldstone bosons of zero momentum. In order to describe this, we enclose the system in a finite box of volume V and replace the integral over k by the corresponding momentum sum

$$\int \frac{d^D k a^D}{(2\pi)^D} \to \frac{a^D}{V} \sum_{k} . \tag{18.79}$$

Since the integrand in (18.67) is singular at $k = 0$, the $k = 0$ mode has to be treated separately. We split the right-hand side of the gap equation (18.68) for $\beta > \beta_c$ as follows

$$1 = N \frac{a^D}{V} \left\{ \frac{1}{\beta \lambda a^2} + \frac{1}{\beta} \sum_{k \neq 0} \frac{1}{\Sigma_{i=1}^D \left[2 - 2\cos(k_i a)\right] + \lambda a^2} \right\}. \tag{18.80}$$

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[4] See pages 390 and 391 in the textbook in Footnote 3.

This equation can now be solved for $\beta > \beta_c$. For $\beta \gg \beta_c$, the very small prefactor a^D/V guarantees a solution with a very small: λa^2 is of the order $a^D/V\beta = a^D/L^D\beta$, where L is the linear size of the system. This follows from the observation that the first nonzero contribution in the sum is of the order

$$\frac{1}{(2\pi a/L)^2 + \lambda a^2} \approx \frac{1}{(2\pi a/L)^2 + \frac{a^D}{L^D}} \tag{18.81}$$

For $D > 2$, one has for large L $a^D/L^D \ll a^2/L^2$, such that the second term in the denominator can be ignored, and the first term in (18.94) is much larger than the second term, which can be neglected. For $\beta > \beta_c$, the gap equation in a large volume reads therefore approximately

$$1 \approx N \frac{a^D}{V\beta\lambda a^2} \tag{18.82}$$

What happens if β is only slightly larger than β_c^2? Since $D > 2$ the sum on the right-hand side can again be replaced by an integral and we find the gap equation, valid for very large V but arbitrary $\beta > \beta_c$:

$$1 \;=\; \frac{a^D}{V}\frac{1}{\beta}\frac{1}{\lambda a^2} + \frac{N}{\beta} v_0(0) = \frac{a^D}{V}\frac{N}{\beta}\frac{N}{\lambda a^2} + \frac{\beta_c}{\beta}. \tag{18.83}$$

Hence the square mass λ of directional fluctuations is found to be

$$\lambda = \frac{1}{N}\frac{a^D}{V}\frac{1}{a^2}\frac{1}{\beta - \beta_c}. \tag{18.84}$$

This is positive and infinitely small for a large volume. As a function of temperature $t = 1/\beta$, this looks very similar to the plot in (18.3).

Let us look in some detail at the difference between the treatment of the gap equation on the lattice and that of the dimensionally regularized gap equation in the continuum field theory. This will allow us to understand the reason for the negative sign of t in the ordered phase in the continuum model. To be specific, we assume $D = 3$. The integral appearing in the gap equation is, in dimensional regularization,

$$\begin{aligned}\int \frac{d^3k}{(2\pi)^3}\frac{1}{k^2+m^2} \;&=\; \bar{S}_D \frac{1}{2}\Gamma\left(\frac{D}{2}\right)\Gamma\left(1-\frac{D}{2}\right) m^{D-2}\Big|_{D=3}\\ &=\; \bar{S}_3 \frac{1}{2}\Gamma\left(\frac{3}{2}\right)\Gamma\left(-\frac{1}{2}\right) m\\ &=\; -\frac{1}{4\pi} m.\end{aligned} \tag{18.85}$$

The corresponding lattice expression is

$$\frac{1}{a^3}\int_{-\pi/a}^{\pi/a} \frac{d^3k a^3}{(2\pi)^3}\frac{1}{a^{-2}\Sigma_i\left[2-2\cos\left(k_i a\right)\right]+m^2} = \frac{1}{a} v^3_{m^2}(0) \tag{18.86}$$

where for small m^2

$$\frac{1}{a}v_0(0) \equiv \frac{1}{4\pi}m + \mathcal{O}(m). \tag{18.87}$$

In the lattice gap equation (18.68), the first term on the right-hand side of (18.94) goes to infinity in the continuum limit $a \to 0$. In the analytic continuation (18.67), on the other hand, it is absent. It is this term which in the lattice model is responsible for the fact that β positive in both phases, with a positive $\beta_c > 0$ separating the two phases. In contrast to this, the two phases in the continuum theory exist for *opposite* signs of the bare quantity β. This curious situation which is caused entirely by the mathematics of analytic regularization is removed after renormalizing the theory. Along the renormalized $1/t_R$ -axis, the situation is again analogous to the more physical one in the lattice model, where β need not be renormalized.

18.7 Background Field Treatment of Cold Phase

There is another more elegant way of dealing with the low temperature phase which does not require the delicate treatment of the $k = 0$ -mode. It yields a consistent gap equation for all temperatures without the intermediate consideration of a finite volume. It is obtained by minimizing the effective action of the model, calculated by expanding n^a around a background field. Let us denote this background field by $N^a(\mathbf{x})$, and the fluctuations around it by $\delta n^a(\mathbf{x}) = n^a(\mathbf{x}) - N^a(\mathbf{x})$. Then the one-loop effective action becomes

$$\begin{aligned}\Gamma[N^a] \;&=\; \frac{N}{2t}\int d^Dx\left\{(\boldsymbol{\nabla}N_a)^2 + \lambda(\mathbf{x})N_a^2(\mathbf{x})\right\}\\ &+\; \frac{N}{2}\mathrm{Tr}\,\log\left[-\boldsymbol{\nabla}^2 - \lambda(\mathbf{x})\right] + \frac{N}{2t}\int d^Dx\,\lambda,\end{aligned} \tag{18.88}$$

to be evaluated at the minimum with respect to $N^a(x)$ and the maximum with respect to λ. In the limit $N \to \infty$, the one-loop effective action $(1/N)\,\Gamma\,[N^a]$ is the exact one.

The new gap equation reads

$$-\frac{{N_a}^2}{t} + \frac{1}{t} = \int \frac{d^Dk}{(2\pi)^D}\frac{1}{\mathbf{k}^2 + \bar{\lambda}} \tag{18.89}$$

and the background field N_a satisfies the equation of motion

$$\left[-\boldsymbol{\nabla}^2 + \bar{\lambda}(\mathbf{x})\right]N_a(\mathbf{x}) = 0. \tag{18.90}$$

This equation shows that $\sqrt{\bar{\lambda}}^{\,-1}$ determines the correlation length of the N_a field. The ground state is obtained for a constant N^a field, which satisfies

$$\bar{\lambda}N_a = 0. \tag{18.91}$$

This has two solutions, $N_a = 0$ or $\bar{\lambda} = 0$. In the first case, the gap equation reduces to the previous one, which in dimensional regularization had a solution only for $t > 0$. In the other phase with $t > 0$, the gap equation turns into an equation for the size of N_a

$$-\frac{N_a^2}{t} + \frac{1}{t} = \int \frac{d^D k}{(2\pi)^D} \frac{1}{\mathbf{k}^2} \tag{18.92}$$

The direction of N_a is arbitrary and will be chosen by the system at will. This shows that for $t > 0$, the ground state displays a spontaneous breakdown of O(N) symmetry. It display a spontaneous magnetization.

Comparison with Eq. (18.47) shows that the gap equation (18.92) coincides precisely with the previous gap equation on the lattice (18.94) for the low temperature phase, with N_a^2/t playing the role of $1/L^D\lambda$. Given the previous solution for $\bar{\lambda}$, we can therefore identify for $t > 0$

$$N_a^2 = \frac{t}{\bar{\lambda}} \frac{1}{L^D}. \tag{18.93}$$

The quantity N_a^2 can be considered as an order parameter of the low temperature phase. It specifies the magnetization $M \equiv \sqrt{N_a^2}$.

In the framework of dimensional regularization, the integral on the right-hand side of the gap equation vanishes and the order parameter for $t_R < t_R^c$ has the value

$$N_a^2 = 1. \tag{18.94}$$

The background vector has the unit lngth of the original fluctuating field $n_a(\mathbf{x})$. The fact that N_a is of unit length for all $t > 0$ or $t_R < t_R^c$ is once more an artifact of dimensional regularization. On a lattice, the magnetization M goes to zero smoothly, with a power law in $\beta - \beta c$:

$$M \propto (\beta - \beta_c)^\beta . \tag{18.95}$$

The power is conventionally denoted by β, which should in thes context not be confused with the inverse temperature β. On a lattice, the gap equation (18.92) reads, for $\beta > \beta_c$,

$$1 - N_a^2 = \frac{N}{\beta} \int_{-\pi/a}^{\pi/a} \frac{d^D k a^D}{(2\pi)^D} \frac{1}{\sum_{i=1}^{D} [2 - 2\cos(k_i a)]}, \tag{18.96}$$

such that

$$1 - N_a^2 = \frac{N v_0^D(\mathbf{0})}{\beta}. \tag{18.97}$$

From this we extract the power behavior

$$M = \sqrt{N_a^2} = \left(1 - \frac{\beta_c}{\beta}\right)^{1/2}, \tag{18.98}$$

showing that the critical exponent β has the value 1/2.

18.8 Quantum Statistics at Nonzero Temperature

Let us also study quantum fluctuations in the non-linear σ-model. For this we assume that one of the spatial coordinates $(x_1, \dots, x_D)$, for instance x_D, is an imaginary time variable τ restricted to the interval $\tau \in (0, \hbar\beta)$ with $\beta = 1/k_BT$, and let the fields be periodic in τ with period $\hbar\beta$. Equivalently, we may think of this model as a nonlinear σ-model on an infinitely long spatial strip with periodic boundary conditions, whose width along the x_D-axis is β. In this context, we shall write the $D-1$ -dimensional purely spatial vectors as fat letters, whereas the D-dimensional spacetime vectors are denoted by slim letters.

Since temperature enters the theory now via the period $\hbar\beta = 1/k_BT$, we shall return to the original notation g for the coupling constant as in the partition function (18.2) [which had been traded for the reduced temperature t in (18.22) and (18.19)]

In the limit $N \to \infty$, we can study the effects of temperature exactly. The partition function is (18.26), and the gap equation has the same form as in (18.27), except that the momentum integral $\int dp_D/2\pi$ is replaced by a sum $T\sum_{p_D=\omega_m}$ over the Matsubara frequencies

$$\omega_m = 2\pi T m, \qquad m = 0, \pm 1, \pm 2, \dots \ . \tag{18.99}$$

guaranteeing the periodicity of the fields on the interval $x_D \in (0, \beta)$. The gap equation (18.27) at finite temperature is therefore

$$\frac{1}{g} = (-\partial^2 + \lambda)^{-1} = \int \frac{d^{D-1}p}{(2\pi)^{D-1}} T \sum_m \frac{1}{{\omega_m}^2 + \mathbf{p}^2 + \lambda}. \tag{18.100}$$

We have gone to natural units with $\hbar = 1$, $k_B = 1$. This equation can be renormalized with the same renormalized coupling constant $g_R(\mu)$ as in the infinite system. We add and subtract, on the right-hand side, the $T = 0$ -limit of the rigth-hand side and obtain

$$\frac{1}{g} - \int \frac{d^D p}{(2\pi)^D} \frac{1}{p^2 + \lambda} = \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \left(T \sum_m \frac{1}{\omega_m^2 + \mathbf{p}^2 + \lambda} - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{\omega^2 + \mathbf{p}^2 + \lambda} \right). \tag{18.101}$$

The left-hand side is the zero-temperature gap equation (18.27).

18.8.1 Two-Dimensional Model

For the subsequent discussion we focus attention on the two-dimensional case. Then the zero-temperature gap equation can be renormalized in $D = 2 + \epsilon$ dimensions using Eq. (18.32). This brings the left-hand side in (18.101) to the form

$$\frac{1}{g} + \bar{S}_D \frac{1}{\epsilon} \mu^\epsilon + \bar{S}_D \frac{\mu^\epsilon}{\epsilon} \left[\left(\frac{\lambda}{\mu^2} \right)^{\epsilon/2} - 1 \right] \approx \frac{1}{g_R(\mu)} + \frac{1}{2} \bar{S}_2 \log \frac{\lambda}{\mu^2}. \tag{18.102}$$

The sum over m on the right-hand side of Eq. (18.177) can be performed using the sum formula

$$T\sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+\Omega^2}=\frac{1}{2\Omega}\coth\frac{\Omega}{2T}, \tag{18.103}$$

with $\Omega\equiv\sqrt{\mathbf{p}^2+\lambda}$. In the limit $T\to 0$, this becomes

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{\omega^2+\Omega^2}=\frac{1}{2\Omega}. \tag{18.104}$$

Subtracting (18.104) from (18.103), and using (18.102), we obtain the temperature-dependent gap equation in two dimensions

$$\frac{1}{g_R(\mu)}+\frac{1}{4\pi}\log\frac{\lambda}{\mu^2}=\int_{-\infty}^{\infty}\frac{dp}{2\pi}\frac{1}{2\Omega}\left(\coth\frac{\Omega}{2T}-1\right). \tag{18.105}$$

Eliminating the arbitrary mass scale μ in favor of the solution $\lambda=\bar{\lambda}$ of this equation for $T=0$, which is

$$\bar{\lambda}=\mu^2e^{4\pi/g_R(\mu^2)}, \tag{18.106}$$

this equation can be rewritten in a renormalization group invariant way as

$$\frac{1}{4\pi}\log\frac{\lambda}{\bar{\lambda}}=\int_{-\infty}^{\infty}\frac{dp}{2\pi}\frac{1}{2\Omega}\left(\coth\frac{\Omega}{2T}-1\right). \tag{18.107}$$

The right hand side is a function of the dimensionless variable λ_T

$$\lambda_T\equiv\lambda/(2\pi iT)^2 \tag{18.108}$$

and will be denoted by

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi}\frac{1}{2\Omega}\left(\coth\frac{\Omega}{2T}-1\right)\equiv\frac{1}{2\pi}S_1(\lambda_T). \tag{18.109}$$

In terms of this function, the gap equation reads simply [compare with the forthcoming fermionic gap function (20.221)]

$$\log\frac{\lambda}{\bar{\lambda}}=2S_1(\lambda_T). \tag{18.110}$$

The functions $S_1(\lambda_T)$ can also be rewritten as follows

$$S_1(\lambda_T)=\int_0^{\infty}\frac{dp}{\Omega}\left[\coth\left(\frac{\Omega}{2T}\right)-1\right]=-2\int_0^{\infty}\frac{dp}{\Omega}\left(1-e^{\Omega/T}\right)^{-1}. \tag{18.111}$$

There exists no critical temperature T_c where λ vanishes.

The gap equation (18.110) is fast convergent only at low temperature.

For high temperatures, it is better to keep the original sum over ω_m in (18.103). Inserting this sum into (18.111), and perform the integral over p gives

$$\begin{aligned} S_1(\lambda_T) &= \pi\left(T\sum_{m=-\infty}^{\infty}-\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\frac{1}{\sqrt{\omega_m^2+\lambda}} \\ &= \frac{1}{2}\left(\sum_{m=-\infty}^{\infty}-\int_{-\infty}^{\infty}dm\right)\frac{1}{\sqrt{m^2+\lambda_T}}. \end{aligned} \tag{18.112}$$

Taking the term with $m=0$ out of the sum, the right-hand side can be rearranged as follows:

$$S_1(\lambda_T)=\frac{1}{2\sqrt{\lambda_T}}+\sum_{m=1}^{\infty}\left(\frac{1}{\sqrt{m^2+\lambda_T}}-\frac{1}{m}\right)+\sum_1^{\infty}\frac{1}{m}-\int_0^{\infty}dm\frac{1}{\sqrt{m^2+\lambda_T^2}}. \tag{18.113}$$

The last two terms diverge. The two divergences cancel each other. To see this we truncate the sum and the integral at some finite large integer value $m=M$. Then the two terms have the limits

$$\sum_{m=1}^{M}\frac{1}{m}\longrightarrow\log M+\gamma+\mathcal{O}\left(\frac{1}{M}\right), \tag{18.114}$$

and

$$\operatorname{arcsin}\frac{M}{\sqrt{\lambda_T}}\longrightarrow\log\frac{2M}{\sqrt{\lambda_T}}+\mathcal{O}\left(\frac{1}{M}\right), \tag{18.115}$$

respectively. Combining them, we obtain the alternative expression for $S_1(\lambda_T)$

$$S_1(\lambda_T)=\tilde{S}_1(\lambda_T)+\frac{1}{2\sqrt{\lambda_T}}+\frac{1}{2}\log\frac{\lambda_T e^{2\gamma}}{4}, \tag{18.116}$$

where $\tilde{S}_1(\lambda_T)$ denotes the convergent sum

$$\tilde{S}_1(\lambda_T)\equiv\sum_{m=1}^{\infty}\left(\frac{1}{\sqrt{m^2+\lambda_T}}-\frac{1}{m}\right). \tag{18.117}$$

Inserting this into (18.116), we arrive at the desired alternative form for the gap equation which converges fast at high temperatures:

$$\log\frac{T}{\bar{T}}=\tilde{S}_1(\lambda_T)+\frac{1}{2\sqrt{\lambda_T}}, \tag{18.118}$$

where $\bar{T}\equiv\sqrt{\bar{\lambda}}e^{\gamma}/4\pi$.

It is straight-forward to calculate $\tilde{S}_1(\lambda_T)$ as a function of λ_T, and find from this $T(\lambda_T)$ as well as $\lambda=\lambda_T\,4\pi^2T$. Plotting $\lambda(T)$ we see that λ starts out with $\bar{\lambda}$ at $T=0$, and grows rapidly to infinity.

The gap equation is obtained by extremizing the effective potential as a function of λ. The effective potential is given by

$$\frac{1}{N}v(\lambda)=\frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}T\sum_m\log(\omega_m^2+\mathbf{p}^2+\lambda)-\frac{\lambda}{2g}. \tag{18.119}$$

We split this again into the zero-temperature equation

$$\begin{aligned}\frac{1}{N}v_0(\lambda) &= \frac{1}{2}\int\frac{d^2p}{(2\pi)^2}\log(p^2+\lambda)-\frac{\lambda}{2g}\\ &= -\frac{\lambda}{8\pi}\left(\log\frac{\lambda}{\bar{\lambda}}-1\right),\end{aligned} \tag{18.120}$$

and a finite temperature correction

$$\begin{aligned}\frac{1}{N}\Delta_T v(\lambda) &= T\int_{-\infty}^{\infty}\frac{dp}{2\pi}\log\left(1-e^{-\Omega/T}\right)\\ &= \frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\left(T\sum_m-\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\log(\omega_m^2+p^2+\lambda).\end{aligned} \tag{18.121}$$

The right-hand side depends only on λ_T, and will be denoted by $(\lambda/2\pi)S_0(\lambda_T)$, i.e.

$$\frac{1}{N}\Delta_T v(\lambda)=\frac{\lambda}{2\pi}S_0(\lambda_T) \tag{18.122}$$

The integral over p in (18.120) can be performed in analytic regularization. For $D=2$, this amounts to the sequence of steps

$$\begin{aligned}\int\frac{dp}{2\pi}\log(\omega_m^2+p^2+\lambda) &= -\int_0^{\infty}\frac{d\tau}{\tau}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\exp[-\tau(\omega_m^2+p^2+\lambda)]\\ &= -\int_0^{\infty}\frac{d\tau}{2\sqrt{\pi}\tau^{3/2}}\exp[-\tau(\omega_m^2+\lambda)]\\ &= -\frac{\Gamma(-1/2)}{2\sqrt{\pi}}\sqrt{\omega_m^2+\lambda}.\end{aligned} \tag{18.123}$$

Hence

$$\begin{aligned}S_0(\lambda_T) &= \frac{\pi}{\lambda}\left(T\sum_{m=-\infty}^{\infty}-\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\sqrt{\omega_m^2+\lambda}\\ &= \frac{1}{2\lambda_T}\left(\sum_{m=-\infty}^{\infty}-\int_{-\infty}^{\infty}dm\right)\sqrt{m^2+\lambda_T}.\end{aligned} \tag{18.124}$$

Note that $S_0(\lambda_T)$ has the derivative

$$\frac{d}{d\lambda_T}\lambda_T S_0(\lambda_T)=\frac{1}{2}S_0(\lambda_T), \tag{18.125}$$

so that a differentiation of the potential

$$\frac{1}{N}v(\lambda) = -\frac{\lambda}{8\pi}\left(\log\frac{\lambda}{\bar{\lambda}} - 1\right) + \frac{\lambda}{2\pi}S_0(\lambda_T) \tag{18.126}$$

leads properly to the gap equation (18.110).

At high temperatures, it is useful to do the same manipulations with $S_0(\lambda_T)$ as with $S_1(\lambda_T)$, and rewriting it as follows

$$S_0(\lambda_T) = \tilde{S}_0(\lambda_T) + \frac{1}{2}\sqrt{\lambda_T} + \frac{1}{4}\left(\log\frac{\lambda_T e^{2\gamma}}{4} - 1\right), \tag{18.127}$$

where

$$\begin{aligned}\tilde{S}_0(\lambda_T) &= \frac{2\pi}{\lambda}T\sum_{m=1}^{\infty}\left(\sqrt{\omega_m^2+\lambda} - \omega_m - \frac{\lambda}{2\omega_m}\right)\\ &= \frac{1}{\lambda_T}\sum_{m=1}^{\infty}\left(\sqrt{\omega^2+\lambda_T} - m - \frac{\lambda_T}{2m}\right).\end{aligned} \tag{18.128}$$

Then the total potential becomes

$$\frac{1}{N}v(\lambda) = -\frac{\lambda}{4\pi}\log\frac{T}{\bar{T}} + \frac{1}{4\pi\sqrt{\lambda_T}} + \frac{\lambda}{2\pi}\tilde{S}_0(\lambda_T). \tag{18.129}$$

In the neighborhood of two dimensions, we set $D = 2+\epsilon > 2$, and split the zero-temperature potential $v_0(\lambda)$ conveniently as follows:

$$\frac{1}{N}v_0(\lambda) = -\frac{\lambda}{2g} - \frac{\lambda}{2}c_\epsilon\frac{1}{1+\epsilon/2}\lambda^{\epsilon/2} = -\frac{\lambda}{2g} - \frac{\lambda\mu^\epsilon}{2}c_\epsilon - \frac{\lambda}{2}c_\epsilon\left[\frac{1}{1+\epsilon/2}\lambda^{\epsilon/2} - \mu^\epsilon\right], \tag{18.130}$$

with c_ϵ of Eq. (18.37) with the small-ϵ behavior (18.38).

The finite-temperature correction can be written as follows:

$$\frac{1}{N}\Delta_T v_T(\lambda_T) = -\frac{\lambda^{D/2}}{2\pi}a_D S_0(\lambda_T), \tag{18.131}$$

with

$$S_0(\lambda_T) = a_D^{-1}\frac{2\pi}{\lambda^{D/2}}\frac{1}{2}\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\left(T\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\log(\omega_m^2+p^2+\lambda), \tag{18.132}$$

where the constant a_D is chosen to have a convenient form for $S_0(\lambda_T)$ at all D:

$$a_D = -\Gamma\left(\frac{1}{2} - \frac{D}{2}\right)\frac{1}{(4\pi)^{(D-1)/2}}, \tag{18.133}$$

with $a_2 = 1$, $a_4 = -1/6\pi$. By rewriting $\log a$ as the analytically regularization integral $-\int_0^\infty (d\tau/\tau)e^{-\tau a}$, Eq. (18.132) becomes

$$\begin{aligned} S_0(\lambda_T) &= -a_D^{-1}\frac{\pi}{\lambda^{D/2}}\left(T\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right) \\ &\times \int_0^\infty \frac{d\tau}{\tau}\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\exp\left(-\tau p^2\right)\exp\left[-\tau(\omega_m^2+\lambda)\right]. \end{aligned} \tag{18.134}$$

The integral over p can now be performed, with the result

$$\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\exp\left(-\tau p^2\right) = (4\pi\tau)^{-(D-1)/2}. \tag{18.135}$$

Using now the integral formula

$$\int_0^\infty \frac{d\tau}{\tau}\tau^{-(D-1)/2}e^{-\tau E} = \Gamma\left(\frac{1-D}{2}\right)E^{(D-1)/2}, \tag{18.136}$$

we find

$$\begin{aligned} S_0(\lambda_T) &= \frac{2\pi}{\lambda^{D/2}}\frac{1}{2}\left(T\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\left(\omega_m^2+\lambda\right)^{(D-1)/2} \\ &= \frac{1}{2{\lambda_T}^{D/2}}\left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}dm\right)(m^2+\lambda_T)^{(D-1)/2} \end{aligned} \tag{18.137}$$

For $D = 2$, this reduces to the previous sum (18.124).

In going from (18.132) to (18.137), we have of course rederived formula (9.133) in the form

$$\int\frac{d^{D-1}q}{(2\pi)^{D-1}}\log(\omega_m^2+q^2) = \frac{1}{(4\pi)^{(D-1)/2}}\Gamma\left(\frac{1}{2}-\frac{D}{2}\right)\sqrt{\omega_m^2}^{\,D-1}, \tag{18.138}$$

18.8.2 Four-Dimensional Model

For $D = 4$, we obtain

$$\begin{aligned} S_0(\lambda_T) &= \frac{\pi}{\lambda^2}\left(T\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\sqrt{\omega_m^2+\lambda}^{\,3} \\ &= \frac{1}{2\lambda_T^2}\left(\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}dm\right)\sqrt{m^2+\lambda_T}^{\,3}. \end{aligned} \tag{18.139}$$

By analogy with the two-dimensional expression (18.127), this can be processed further to a convergent sum

$$\tilde{S}_0(\lambda_T) = \frac{1}{\lambda_T^2}\sum_{m=1}^{\infty}\left\{\sqrt{m^2+\lambda_T}^{\,3} - m^3 - \frac{3}{2}\lambda_T m - \frac{3}{8}\frac{\lambda_T^2}{m}\right\}. \tag{18.140}$$

18.8.3 Any Dimension

In any dimension D, the expression $a^D S_0(\lambda_D)$ in temperature correction (18.131) to the potential which generalizes (18.127) is derived as follows: First we perform the integral over ω_m in (18.137), and rewrite $a^D S_0(\lambda_T)$ as

$$a^D S_0(\lambda_T) = a_D \frac{1}{{\lambda_T}^{D/2}} \left[\lambda_T^{(D-1)/2} + 2 \sum_{m=1}^{\infty} (m^2 + \lambda_T)^{(D-1)/2} \right] + \pi c_\epsilon \frac{2}{D}, \tag{18.141}$$

the last term coming from the integral over ω_m in (18.137) [recall (18.37)]. Then we expand the second term in powers of λ_T as

$$a^D S_0(\lambda_T) = a_D \frac{1}{{\lambda_T}^{D/2}} \left[\lambda_T^{(D-1)/2} + 2 \sum_{m=1}^{\infty} \sum_{k=0}^{\infty} \begin{pmatrix} (D-1)/2 \\ k \end{pmatrix} m^{D-1-2k} \lambda_T^k \right] + \pi c_\epsilon \frac{2}{D}. \tag{18.142}$$

Performing the sum over m in the curly brackets gives

$$\left[\lambda_T^{(D-1)/2} + 2 \sum_{k=0}^{\infty} \begin{pmatrix} (D-1)/2 \\ k \end{pmatrix} \zeta(2k+1-D) \lambda_T^k \right]. \tag{18.143}$$

For an even dimension $D = \bar{D}$, the term with $k = \bar{D}/2$ has a singularity for D close to 2, 4, … . This singularity cancels a corresponding one in c_ϵ.

Let D be close to the even dimension $\bar{D}$, say $D = \bar{D} + \epsilon$. Then there are two singular terms in $a_D S_0(\lambda_T)$:

$$\begin{aligned} a_D S_0(\lambda_T)\Big|_{\text{sg}} \;=\; & -\Gamma\left(\frac{1}{2} - \frac{D}{2}\right) \frac{1}{\sqrt{4\pi}^{D-1}} \frac{1}{\lambda_T^{D/2}} \frac{\Gamma\left(\frac{1}{2} + \frac{D}{2}\right)}{\Gamma\left(\frac{\bar{D}}{2} + 1\right) \Gamma\left(\frac{1}{2} + \frac{\epsilon}{2}\right)} \zeta(1-\epsilon) \lambda_T^{\bar{D}/2} \\ & - \frac{1}{2\sqrt{4\pi}^{D-2}} \Gamma\left(1 - \frac{\bar{D}}{2} - \frac{\epsilon}{2}\right) \frac{1}{\bar{D} + \epsilon}. \end{aligned} \tag{18.144}$$

Expanding $\zeta(1-\epsilon) = -(1-\epsilon\gamma)/\epsilon + \ldots$, the $1/\epsilon$-singularity in the first term is given by

$$\frac{1}{\sqrt{4\pi}^{\bar{D}-1}} \Gamma\left(\frac{1}{2} - \frac{\bar{D}}{2}\right) \frac{\Gamma\left(\frac{1}{2} + \frac{\bar{D}}{2}\right)}{\Gamma\left(\frac{\bar{D}}{2} + 1\right) \Gamma\left(\frac{1}{2}\right)} \frac{1}{\epsilon} = \frac{1}{\sqrt{4\pi}^{\bar{D}-1}} \frac{(-)^{\bar{D}/2}}{\Gamma\left(\frac{\bar{D}}{2}\right) \frac{\bar{D}}{2} \epsilon}. \tag{18.145}$$

In the second term, we write

$$\Gamma\left(\frac{1}{2} - \frac{\bar{D}}{2} - \frac{\epsilon}{2}\right) = (-)^{\bar{D}/2} \frac{\Gamma(1+\epsilon/2)}{\Gamma\left(\bar{D}/2 + \epsilon/2\right)} \frac{2}{\epsilon} \Gamma(1-\epsilon/2) = \frac{(-1)^{\bar{D}/2} \pi}{\Gamma\left(\frac{\bar{D}}{2} + \frac{\epsilon}{2}\right) \sin\frac{\pi\epsilon}{2}}, \tag{18.146}$$

and see that the $1/\epsilon$-singularities cancel each other. The finite-ϵ independent contribution is obtained by expanding

$$\Gamma(k+\epsilon)=\Gamma(k)[1+\epsilon\psi(k)], \tag{18.147}$$

such that the first $1/\epsilon$ -singularity is accompanied by

$$\left\{1+\frac{\epsilon}{2}\left[-\log\lambda_T-\psi\left(\frac{1}{2}-\frac{\bar{D}}{2}\right)+\psi\left(\frac{1}{2}+\frac{\bar{D}}{2}\right)-\psi\left(\frac{1}{2}\right)-2\gamma-\log 4\pi\right]\right\}. \tag{18.148}$$

The second singularity has a residue

$$\left\{1+\frac{\epsilon}{2}\left[-\log 4\pi-\frac{2}{\bar{D}}-\psi\left(\frac{\bar{D}}{2}\right)\right]\right\}. \tag{18.149}$$

Since

$$\psi\left(\frac{1}{2}+\frac{\bar{D}}{2}\right)-\psi\left(\frac{1}{2}-\frac{\bar{D}}{2}\right)=\pi\cot\frac{\pi\bar{D}}{2}=0,$$

the difference is

$$-\frac{\epsilon}{2}\left(\log\frac{\lambda_T e^{2\gamma}}{4}-\sum_{k=1}^{\bar{D}/2}\frac{1}{k}\right). \tag{18.150}$$

Thus, altogether, we obtain for an even numbers of dimension $D=2,4,6,\ldots$ the finite sums

$$S_0(\lambda_T)=\frac{1}{2\lambda_T^{D/2}}\left[\lambda_T^{(D-1)/2}+2\sum_{k=0,\neq D/2}^{\infty}\binom{(D-1)/2}{k}\zeta(2k+1-D)\lambda_T^k\right]+S_0^L(\lambda_T), \tag{18.151}$$

where

$$S_0^L(\lambda_T)\equiv-\frac{a_D^{-1}(-)^{D/2}}{4\Gamma\left(1+\frac{D}{2}\right)}\frac{1}{\sqrt{4\pi}^{D-2}}\left[\log\left(\frac{\lambda_T}{4e^{-2\gamma}}\right)-\sum_{k=1}^{D/2}\frac{1}{k}\right]. \tag{18.152}$$

It is now easy to split (18.151) into

$$S_0(\lambda_T)=\tilde{S}_0(\lambda_T)+\frac{1}{2\sqrt{\lambda_T}}+\tilde{S}_0(\lambda_T)+\tilde{\tilde{S}}_0(\lambda_T)+S_0^L(\lambda_T) \tag{18.153}$$

with the convergent sum

$$\tilde{S}_0(\lambda_T)=\frac{1}{\lambda_T^{D/2}}\sum_{k=D/2+1}^{\infty}\binom{(D-1)/2}{k}\zeta(2k+1-D)\lambda_T^k, \tag{18.154}$$

and the finite sum

$$\tilde{\tilde{S}}_0(\lambda_T)=\frac{1}{\lambda_T^{D/2}}\sum_{k=0}^{D/2-1}\binom{(D-1)/2}{k}\zeta(2k+1-D)\lambda_T^k. \tag{18.155}$$

Inserting the the divergent representation $\sum_{m=1}^{\infty} m^{-z}$ for the ζ-function at negative z, this is formally equal to the divergent sum

$$\tilde{\tilde{S}}_0(\lambda_T) = \frac{1}{\lambda_T^{D/2}} \sum_{m=0}^{\infty} \left(m^{D-1} + \frac{D-1}{2} \lambda_T m^{D-3} + \dots \right), \tag{18.156}$$

where the last omitted term in parentheses is proportional to $\lambda_T^{D/2-1}/m$. The convergent sum (18.154) is obviously equal a convergent power series expansion of the convergent infinite series

$$\tilde{S}_0(\lambda_T) = \frac{1}{2\lambda_T^{D/2}} \sum_{m=1}^{\infty} \left(\sqrt{m^2+\lambda_T}^{\,D-1} - m^{D-1} - \frac{D-1}{2} \lambda_T m^{D-3} + \dots \right), \tag{18.157}$$

where as many powers of λ_T are subtracted as needed for convergence. These are the generalizations of the two- and four-dimensional expressions (18.128) and (18.140), respectively. The expression (18.153) written in this way converges fast for high temperatures.

Let us now derive an expression which converges fast at low temperature T. For this it is most convenient to use the D-dimensional generalization of Eq. (18.121)

$$\begin{aligned} \frac{1}{N} \Delta_T v(\lambda) &= \frac{1}{2} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \left(T \sum_m - \int_{-\infty}^{\infty} \frac{d\omega_m}{2\pi} \right) \log(\omega_m^2 + p^2 + \lambda) \\ &= T \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \log\left(1 - e^{-\Omega/T}\right). \end{aligned} \tag{18.158}$$

and expand the logarithm in powers of $e^{-\Omega/T}$. This gives

$$\frac{\lambda^{D/2}}{2\pi} a_D S_0(\lambda_T) = -T \sum_{\tilde{m}=1}^{\infty} \frac{1}{\tilde{m}} \int \frac{dp^{D-1}}{(2\pi)^{D-1}} e^{-\tilde{m}\sqrt{p^2+\lambda}/T} \tag{18.159}$$

$$= -\frac{1}{2\pi} S_{D-1} \lambda^{D/2} \frac{1}{\sqrt{\lambda_T}} \sum_{\tilde{m}=1}^{\infty} \frac{1}{\tilde{m}} \int_0^{\infty} dss^{D-2} e^{-\tilde{m}\sqrt{\lambda})\sqrt{s^2+1}/T}.$$

We now use the integral formula

$$K_\nu(z) = \left(\frac{z}{2}\right)^{\nu} \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\nu+\frac{1}{2}\right)} \int_0^{\infty} dss^{2\nu} \left(s^2+1\right)^{-1/2} e^{-z\sqrt{s^2+1}}, \tag{18.160}$$

and see that

$$S_0(\lambda_T) = 2\pi \frac{2^{D/2}}{\Gamma\left(\frac{1}{2}-\frac{D}{2}\right)\Gamma\left(\frac{1}{2}\right)} \sum_{\tilde{m}=1}^{\infty} \frac{1}{\left(2\pi\tilde{m}\sqrt{\lambda_T}\right)^{D/2}} K_{D/2}\left(2\pi\tilde{m}\sqrt{\lambda_T}\right). \tag{18.161}$$

The same expression will be found once more in an exactly solvable fermionic model in Eq. (20.273), except for a fermionic alternating sign $(-)^{\tilde{m}-1}$.

For $D=2$, the sum (18.161) reduces to

$$S_0(\lambda_T) = -2\sum_{\tilde{m}=1}^{\infty}\frac{1}{2\pi\tilde{m}\sqrt{\lambda_T}}K_1\left(2\pi\sqrt{\lambda_T}\tilde{m}\right) \tag{18.162}$$

we can take the limit of large T, using $K_1(z) \underset{z\to 0}{\longrightarrow} 1/z$, and find

$$S_0(\lambda_T) \xrightarrow{T\to\infty} -\frac{1}{2\pi^2\lambda_T}\sum_{\tilde{m}=1}^{\infty}\frac{1}{\tilde{m}^2} = -\frac{1}{2\pi^2\lambda_T}\zeta(\omega) = -\frac{1}{12\lambda_T}. \tag{18.163}$$

This yields the free energy of black-body radiation in two dimensions

$$\frac{1}{N}\Delta_T v(\lambda) \underset{T\to\infty}{\longrightarrow} -T^2\frac{\pi}{6}. \tag{18.164}$$

The same result could have been obtained from the divergent expression (18.119) using the generalized Euler-Maclaurin formula [regularized by analytic continuation as in the formal calculation of the Casimir effect in Eq. (5.693)]

$$\begin{aligned}\frac{1}{N}\Delta_T v(\lambda) &= \frac{1}{2}\int\frac{dp}{2\pi}T\left[\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right]\log(\omega_m^2+p^2)\\ &= \frac{1}{2}T\sum_{m=-\infty}^{\infty}\sqrt{\omega_m^2} = 2\pi T^2\zeta(-1) = -T^2\frac{\pi}{6}.\end{aligned} \tag{18.165}$$

In the second step we have used the integral formula (9.133) in the form

$$\int\frac{d^{D-1}q}{(2\pi)^{D-1}}\log(\omega_m^2+q^2) = \frac{1}{(4\pi)^{(D-1)/2}}\Gamma\left(\frac{1}{2}-\frac{D}{2}\right)\sqrt{\omega_m^2}^{\,D-1}, \tag{18.166}$$

In four dimensions, we have

$$S_0(\lambda_T) = 6\sum_{\tilde{m}=1}^{\infty}\frac{1}{\left(2\pi\tilde{m}\sqrt{\lambda_T}\right)^2}K_2\left(2\pi\tilde{m}\sqrt{\lambda_T}\right) \tag{18.167}$$

which becomes for large T [using $K_2(z) \underset{z\to 0}{\longrightarrow} 2/z^2$]

$$S_0(\lambda_T) \xrightarrow{T\to\infty} 12\sum_{\tilde{m}=1}^{\infty}\frac{1}{\left(2\pi\tilde{m}\sqrt{\lambda_T}\right)^4} = \frac{12T^4}{\lambda^2}\zeta(4) = \frac{12}{\lambda^2}T^4\frac{\pi^4}{90}. \tag{18.168}$$

The potential

$$\frac{1}{N}\Delta_T v = \frac{\lambda^2}{12\pi^2}S_2 = -T^4\frac{\pi^2}{90} \tag{18.169}$$

is the analog of the free energy density f of black-body radiation. It is related to the internal energy density. u by $f=-\frac{1}{3}u$.

Recall the analog of the *Stephan-Boltzmann law* for the free energy density f of hot (or massless) bosons. In this limit, f has a pure power behavior of T^n, and the associated entropy density $s = -\partial f/\partial T$ is related to f by a factor $-4/T$. For the internal energy density $u \equiv E/V = f + TS$ and for the specific heat at constant volume $c_V = \partial u/\partial T|_V$, the factors are $1 - n$ and $(1 - n)n/T$, respectively.

The original Stefan-Boltzmann law for black body radiation is obtained from this by accounting for the two polarization degrees of freedom with an extra factor 2 so that

$$\Delta_T v = f = -\frac{1}{3}u = -2\frac{\pi^2 T^4}{90}. \tag{18.170}$$

In physical units, this becomes

$$f = -2\frac{2}{3}\frac{\sigma}{c}T^4, \tag{18.171}$$

where σ is the *Stephan-Boltzmann constant*

$$\sigma = \frac{\pi^2 k_B^4}{60\hbar^3 c^2} \approx 5.67 \times 10^{-5} \frac{\text{g}}{\sec{}^\circ\text{K}^4} \tag{18.172}$$

The same result could, of course have been obtained directly from (18.132), which leads to the four-dimensional version of Eq. (18.165). Using (18.166) for $D = 3$ we obtain

$$\begin{aligned}\frac{1}{N}\Delta_T v(\lambda) &= \frac{1}{2}\int \frac{d^3p}{(2\pi)^3} T\left[\sum_{m=-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right]\log(\omega_m^2 + p^2)\\ &= \frac{1}{2}T\sum_{m=-\infty}^{\infty}\frac{1}{(4\pi)^{3/2}}\frac{2}{3}\Gamma(-1/2)\sqrt{\omega_m^2}^{\,3} = -\frac{4}{3\pi}T^4\zeta(-3) = -T^4\frac{\pi^2}{90}.\end{aligned} \tag{18.173}$$

recalling Eq. (5.694).

At arbitrary D, we use the small-z behavior

$$K_\nu(z) \approx \frac{1}{2}\left(\frac{2}{z}\right)^\nu \Gamma(\nu),$$

in (18.161) to find

$$\begin{aligned}S_0(\lambda_T) \quad &\xrightarrow{T\to 0} \quad -a_D^{-1} 2\pi^{1-D/2}\Gamma\left(\frac{D}{2}\right)\frac{1}{\left(2\pi\sqrt{\lambda_T}\right)^D}\zeta(D)\\ &= \quad -\frac{2\pi}{\lambda^{D/2}a_D}\frac{1}{\pi^{D/2}}\Gamma\left(\frac{D}{2}\right)T^D\zeta(D).\end{aligned} \tag{18.174}$$

Dropping the prefactor factor $2\pi/\lambda^{D/2}a_D$ gives the finite-temperature contribution $\Delta_T v(\lambda)/N$ to the free energy density in D dimensions.

$$\Delta_T v(\lambda)/N \quad \xrightarrow{T\to\infty} \quad -\frac{1}{\pi^{D/2}}\Gamma\left(\frac{D}{2}\right)T^D\zeta(D). \tag{18.175}$$

The same result could, of course, have been obtained directly from (18.132), using

$$\sum_{m=-\infty}^{\infty} \omega_m^{D-1} = (2\pi T)^{D-1} 2\zeta(1-D), \tag{18.176}$$

and the well-known identity for Riemann's ζ-functions[5]

$$\Gamma\left(\frac{1}{2}-\frac{z}{2}\right)\zeta(1-z) = \pi^{1/2-z}\Gamma\left(\frac{z}{2}\right)\zeta(z). \tag{18.177}$$

18.9 Criteria for Onset of Fluctuations in Ginzburg-Landau Theories

The understanding of the nonlinear σ-model permits us to improve our understanding of the phase transition in ϕ^4-theories with O(N)-symmetry discussed in Chapter 15. We shall base the discussion on the euclidean version of the Lagrangian (15.6), which is then called *Ginzburg-Landau* Hamiltonian [1]:

$$\mathcal{H}(\phi_a, \partial\phi_a) = \frac{1}{2}\left(\partial\phi_a\right)^2 + \frac{m^2}{2}\phi_a^2 + \frac{g}{4}\left(\phi_a^2\right)^2. \tag{18.178}$$

In the associated partition function

$$Z = \int \mathcal{D}\phi_a e^{-\int d^Dx \mathcal{H}/k_BT}, \tag{18.179}$$

a phase transition takes place at a temperature T_c which lies always *below* the mean field temperature $T_c^{\rm MF}$, where the mass term in (18.178) changes its sign. It is possible to give a rough estimate of the shift $\Delta T \equiv T_c^{\rm MF} - T_c$ which is caused by fluctuations.

After an obvious renormalization of field and mass, the Ginzburg-Landau energy density in D dimensions may be written as

$$\mathcal{H}(\phi_a,\partial\phi_a) = \frac{1}{2a^D}\left\{\alpha^2 a^2[\partial\phi_a(x)]^2 + \tau\phi_a^2(x) + \frac{g}{2}\left[\phi_a^2(x)\right]^2\right\}. \tag{18.180}$$

From here on we use natural units with $k_BT_c^{\rm MF} = 1$. The fields have zero engineering dimension, a denotes some microscopic length scale of the system, usually the size of atoms or molecules, and g is some interaction strength. The parameter α specifies the zero-temperature coherence length of the system in units of a as being $\xi_0 = \alpha a/\sqrt{2}$. This can vary greatly from system to system. In superconductors, for example, α it can lie anywhere between a few thousand, and less than ten in high-temperature superconductors.

We shall here only be concerned with the destruction of the ordered state which lies *below* the critical temperature where $\tau < 0$: There the fields in the energy density fluctuate around an ordered ground state with a constant vector $\langle\phi_a\rangle \equiv \Phi_a \equiv \langle\phi\rangle N_a \equiv \Phi N_a$ in field space, whose direction vector N_a breaks spontaneously the O(N)-symmetry, and whose magnitude is $\Phi = \sqrt{\Phi_a^2} = \sqrt{-\tau/g}$, where the energy density is minimal, fluctuating around the condensation energy density $\mathcal{H}_0 = \mathcal{H}(\Phi_a, 0) = -\tau^2/4ga^D$. The temperature-dependent coherence length $\xi = \alpha a/\sqrt{2|\tau|}$ describes the range of the size fluctuations of the order field.

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[5] See, for instance, I.S. Gradsteyn and I.M. Ryznik, *Table of Integrals, Series, and Products*, Academic Press, New York, 1980, formula 9.635.4.

18.9.1 Ginzburg's Criterion

The magnitude of the fluctuations is estimated by assuming the field to live in patches on a simple cubic lattice of spacing $\xi_l = l\xi$, choosing eventually a spacing parameter between $l = 1$ and 2 to ensure the independence of the patches. In the low-temperature ordered phase with $\tau < 0$, the small fluctuations $\delta\phi(x) = \phi(x) - \Phi$ of the size of the order field $\phi(x)$ around the minimum of (18.180) have an Hamiltonian

$$\mathcal{H}_{\rm sz}(\phi_a,\partial\phi_a) \equiv \frac{1}{2a^D}\left\{\alpha^2a^2[\partial\phi(x)]^2 + 2|\tau|\delta\phi^2(x)\right\}. \tag{18.181}$$

Their size is therefore given by

$$\langle[\phi(x)-\Phi]^2\rangle = \int\frac{d^Dk}{(2\pi)^D}\frac{a^D}{\alpha^2a^2k^2+2|\tau|} = \frac{a^{D-2}}{\xi_l^{D-2}}\frac{1}{\alpha^2}\int\frac{d^Dq}{(2\pi)^D}\frac{1}{q^2+l^2}, \tag{18.182}$$

where q is the dimensionless reduced momentum $\xi_l k$. Inserting ξ_l, the right-hand side can be rewritten as

$$\frac{l^{2-D}}{\alpha^D}(2|\tau|)^{D/2-1}\int\frac{d^Dq}{(2\pi)^D}\frac{1}{q^2+l^2}, \tag{18.183}$$

The relative size of the fluctuations can therefore be written as

$$\frac{\langle[\phi(x)-\Phi]^2\rangle}{\Phi^2} = 2l^{2-D}(2|\tau|)^{D/2-2}g\alpha^{-D}v_{l^2}^D(0), \tag{18.184}$$

where $v_{l^2}^D(0)$ is the lattice Yukawa potential of reduced mass l of Eq. (18.67). Its size is calculated most easily with the help of the integral formula (18.72). Mean-field behavior breaks down if (18.184) is of the order unity, which happens at the reduced Ginzburg temperature

$$|\tau_G| \approx [l^{2-D}K\,v_{l^2}^D(0)]^{2/(4-D)}, \qquad D < 4. \tag{18.185}$$

where

$$K \equiv 2^{D/2-1}g/\alpha^D, \tag{18.186}$$

i.e., at a Ginzburg temperature $T_G \equiv T_c^{\rm MF}(1-|\tau_G|)$. Ginzburg, in his original paper [2], estimated $l \approx 1$ and $v_1^D(0)$ in three dimensions by an integral carried up to $|p| = \pi$:

$$v_1^D(0) \approx \int\frac{d^3p}{(2\pi)^3}\frac{1}{p^2+1} \approx \frac{1}{2\pi^2}\int_0^\pi dp\,p^2\frac{1}{p^2+1} \approx \frac{1}{4\pi}. \tag{18.187}$$

This led him to the estimate

$$|\tau_G| \approx \frac{1}{8\pi^2}\frac{g^2}{\alpha^3}. \tag{18.188}$$

In old-fashioned type-II superconductors, $|\tau_G|$ can be as small as 10^{-8} [3], which explains why conventional superconductors are well described by mean-field theory. In modern high-T_c superconductors, on the other hand, Ginzburg's estimate leads to $|\tau_G| \approx 0.01$ [4], such that critical exponents become observable.

The length parameter l is a free parameter this criterium and Landau's estimate based on the assumtion $l \approx 1$ corresponds to the physical situation that the order field $\Phi(\mathbf{x}$ is properly defined only up to a length scale of the order of the coherence length. In an ordinary superconductor, this is indeed the case. There the order field describes the Cooper pairs of electrons whose wave function extends over a coherence length, such that the cutoff in all momentum integrals would be of this order. In modern superconductors, where the phase transition occurs at higher critical temperature of the order of 100 K, however, the Cooper pairs could have a much smaller diameter than the coherence length.[6] In this case, l would be considerably smaller than unity. If the Cooper pairs are bound very strongly, another effect appears: The phase transition is caused by quantum fluctuations. In this limit, the Cooper pairs form an almost free gas of almost point-like bosons which undergo Bose-Einstein condensation of the type described in Subsection 2.14.3. The relevant length scale is then the De Broglie wavelength of thermal motion

$$\lambda = \frac{2\pi\hbar}{\sqrt{2Mk_BT}}, \tag{18.189}$$

where M is the mass of the Cooper pairs.

For $D > 4$, the right-hand side in (18.184) decreases when approaching the critical point, so only mean-field behavior is observed. If $D = 4-\varepsilon$ lies only slightly below four, the right-hand side of (18.184) behaves like $|\tau|^{-\varepsilon/2}$, implying a good mean-field description until $|\tau|$ is extremely small.

18.9.2 Kleinert's Criterion

If a ϕ^4-theory has only a single real field, Ginzburg's criterion gives a reliable estimate at which temperature fluctuations become important. In an O(N)-symmetric system with Nambu-Goldstone modes, however, it grossly underestimated the temperature shift ΔT of the transition. A better estimate is based on the observation that the kinetic term defines a second, completely independent, energy scale of the system. To identify it, we split the fields according to size and direction in O(N) field space as $\phi_a = \phi n_a$, $n_a^2 = 1$. The directions n_a describe the long-range fluctuations of the Goldstone modes. Sufficiently far from the critical regime, we may neglect the gradient term of the size $\phi(x)$, and approximate the energy density by

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[6] See E. Babaev and H. Kleinert, Phys. Rev. B *59*, 12083 (1999) (cond-mat/9907138), and references therein.

$$\mathcal{H}(\phi, \partial n_a) = \frac{1}{2a^D}\left\{\alpha^2 a^2 \phi^2(x)\,[\partial n_a(x)]^2 + \tau\phi^2(x) + \frac{g}{2}\phi^4(x)\right\}.$$

The fluctuations of the Goldstone modes are controlled by the gradient term whose magnitude depends on the size Φ of ϕ at the minimum of the potential. The gradient energy density is

$$\mathcal{H}_{n_a}(\partial n_a) = \frac{\beta}{2\xi_l^{D-2}}[\partial n_a(x)]^2, \tag{18.190}$$

with

$$\beta = \beta(\Phi) = \alpha^2\left(\frac{\xi_l}{a}\right)^{D-2}\Phi^2 = \frac{\alpha^D l^{D-2}}{2(2|\tau|)^{D/2-2} g} = \frac{1}{K}\frac{l^{D-2}}{|\tau|^{D/2-2}}. \tag{18.191}$$

This is the second energy scale. It measures how much energy is spent when reversing the direction vector n_a over the distance ξ_l. It is the continuous version of the *stiffness* of the directional field defined for a lattice model in Eq. (18.64).

From the discussion of the spherical model in Section 18.6 we know that directional fluctuations disorder a system if the bending stiffness drops below a certain critical value $\beta_{\rm cr}$. For the O(N)-symmetry with large N, this critical value was found to be, on a cubic lattice, in three, four, and large-D dimensions [see Table 18.1 and the hopping expansion (18.74)]

$$\beta_{\rm cr} = N v_0^D(0) \approx N\,0.2527, \quad N\,0.1549, \quad N/2D, \tag{18.192}$$

respectively. We have remarked below Eq. (18.76) that, although these values were derived only for large N, Monte Carlo simulations show they can be trusted already for $D = 3$ and $N = 2$ to within about 10%.

The simulations are done by putting the Heisenberg model on a lattice of unit spacing, so that the energy density for $N = 2$ takes the XY-model form

$$\mathcal{H}_{XY}(\partial n_a) \approx \beta \sum_{\mu=1,\dots,D} [1 - \cos\nabla_\mu \gamma(x)], \tag{18.193}$$

where ∇_i denotes the lattice gradient in the ith coordinate direction, and $\gamma \equiv \arctan n_2/n_1$. Since the quality of the approximation increases with N and D, we can trust Eq. (18.192) to within 10% for *all* N and $D \geq 3$. his accuracy will be sufficient for the criterion to be derived here.

The critical stiffness can, incidentally, be also estimated by calculating its renormalized version from a sum of an infinite number of terms in a perturbation expansion. Expanding the cosine in the energy (18.193) into a Taylor series, and calculating the harmonic expectation values of quartic, sextic, etc. terms, we find in a self-consistent approximation of the Hartree-Fock-Bogoliubov type that the stiffness has a renormalized value [7] $\beta_R = \beta\, e^{-1/2D\beta_R}$. This softens with increasing temperature $1/\beta$, until β reaches a critical value $\beta_{\rm cr} = e/2D$, where β_R drops to zero. In $D = 3$ dimensions, this happens at $\beta_{\rm cr} = 0.4530\dots$, a value which is in excellent agreement with the Monte Carlo number $\beta_{\rm cr}^{\rm MC} \approx 0.45$. The prediction of such sharp drop is true only in two dimensions, as shown by Kosterlitz and Thouless [6]. For $D > 2$ it is an artefact of the approximations, and the exact stiffness goes to zero like $|T_c - T|^{(D-2)\nu}$, with a critical exponent $\nu \approx 1/2 + (4-D)/10 + \dots$.

The estimate for the critical stiffness (18.192) leads now directly to the announced criterion: The phase fluctuations will disorder the system if the stiffness β in Eq. (18.190) drops below the critical value (18.192), which happens at a reduced temperature

$$|\tau_K| \approx [Nl^{2-D}K\,v_0^D(0)]^{2/(4-D)}, \qquad D < 4,\ N \geq 2. \tag{18.194}$$

Thus we obtain the important result that

$$|\tau_K| \approx [Nv_0^D(0)/v_{l^2}^D(0)]^{2/(4-D)}|\tau_G|, \quad D < 4,\ N \geq 2. \tag{18.195}$$

This implies that for all systems with $N \geq 2$, directional fluctuations destroy the order *before* size fluctuations become large. They cause a phase transition below the Ginzburg temperature, at $T_K \equiv T_c^{\rm MF}(1 - |\tau_K|)$. For $D = 3$, and $l = (1, 3/2, 2)$, the relation becomes $|\tau_K| \approx N^2|\tau_G| \times (2.20, 3.48, 5.56)$. Thus, if the critical regime is approached in a ϕ^4-theory with a well-formed mean-field regime, the transition is *always* initiated by directional fluctuations. In particular, the estimates for the critical regime of the high-$|T_c|$ superconductors [4] will receive a factor ≈ 9.

The dominance of directional fluctuations is, of course, most prominent in the limit of large N, and it is therefore not surprising that the critical exponents of the ϕ^4-theory and the Heisenberg model have the same $1/N$-expansions in any dimension $D > 2$, as a pleasant demonstration of the universality of critical phenomena.

By adding to the field energy density $\mathcal{H}(\phi, \partial n_a)$ the energy density of directional fluctuations with the field-dependent stiffness $\beta = \beta(\phi) = \alpha^D\phi^2 l^{D-2}/(2|\tau|)^{D/2-1}$ we can study, as in Ref. [8], the combined energy density in the disordered phase where the symmetry is restored but the average Φ of the size of the order field ϕ is nonzero.

The directional fluctuations play a crucial role in pion physics, as pointed out in Ref. [8] and discussed in detail in Section 20.10.

18.9.3 Experimental Consequences

How do we determine experimentally the fluctuation parameter K to estimate $|\tau_G|$ and $|\tau_K|$? In magnetic systems, one measures the susceptibility tensor $\chi_{AB}(k) \equiv \int d^Dx e^{ikx}\langle\phi_a(x)\phi_b(0)\rangle$ at wave vector k, and decomposes it into parallel and perpendicular parts as $\chi_{AB}(k) = (\Phi_a\Phi_b/\Phi^2)\chi_{\|}(k) + (\delta_{AB} - \Phi_a\Phi_b/\Phi^2)\chi_{\perp}(k)$. The mean-field behavior of these quantities is $\chi_{\|}(k) \approx a^D/(\alpha^2a^2k^2 + 2|\tau|)$ and $\chi_{\perp}(k) \approx a^D/\alpha^2a^2k^2$. Combining these at $k = 0$ with the mean-field behavior of the spontaneous magnetization $\Phi = \sqrt{|\tau|/g}$, and with the temperature-dependent coherence length ξ, we see that the size of K can immediately be estimated from a plot, versus $t \equiv T/T_c - 1$, of either of the dimensionless experimental quantities

$$K_{\rm exp} \;\approx\; |t|^{2-D/2}\frac{k^2}{\xi^{D-2}}\frac{\chi_\perp(k)}{k_BT\Phi^2}\bigg|_{k\to0}, \tag{18.196}$$

or

$$K_{\rm exp} \;\approx\; |t|^{2-D/2}\frac{1}{\xi^{D}}\frac{\chi_{\|}(0)}{k_BT\Phi^2}, \tag{18.197}$$

these being written down in physical units. Note that t measures the temperature distance from the experimental T_c, in contrast to $\tau \equiv T/T_c^{\rm MF} - 1$. In the mean-field regime, where $t \approx \tau$, $K_{\rm exp}$ is constant, and can be inserted into Eq. (18.194) to find the temperature T_K where directional fluctuations destroy the order.

In superfluid helium we may plot, in analogy to the transverse susceptibility expression for $K_{\rm exp}$, the quantity $K_{\rm exp} \approx |t|^{2-D/2}M^2k_BT/\xi^{D-2}\hbar^2\rho_s$, where M is the atomic mass and ρ_s the superfluid mass density, which at the mean-field level is defined by writing the gradient energy (18.190) as e gradient energy (18.190) as $(\rho_s/2k_BT)(\hbar^2/M^2)[\partial n_a(x)]^2$. In the critical regime, the three expressions for $K_{\rm exp}$ go universally to zero like $|t|^{2-D/2}$, since $\xi \propto |t|^{-\nu}$, $\chi_{\|}(0) \approx |t|^{(\eta-2)\nu}$, $k^2\chi_\perp(k)|_{k\to0} \approx |t|^{\eta\nu}$, $\Phi^2 \approx |t|^{\nu(D-2+\eta)}$, $\rho_s \approx |t|^{(D-2)\nu}$, with $\eta \approx [(N+2)/2(N+8)^2](4-D)^2 + \dots$.

Experimentally, the superfluid density of helium for $D = 3$ shows no mean-field behavior a la Ginzburg-Landau down to $T \approx T_c/4$, such that the above formulas cannot properly be applied. Let us nevertheless estimate orders of magnitude of a would-be mean-field behavior: $\rho_s/\rho \approx 2|\tau|$ [9], where $\rho = M/a^3$ is the total mass density, with $a \approx 3.59\,$Å [10]. Then the factor k_BT_c at $T_c = 2.18\,$K can be expressed as $k_BT_c \approx 2.35\hbar^2/Ma^3$ [10]. With $\xi_0 \approx 2\,$Å, we obtain an estimate $K \approx 1.2\,a/\xi_0 \approx 2$. Inserting this into Eq. (18.194) and relation (18.195), we obtain for $l = 1$ and 2

$$|\tau_K| \approx 1,\;\; |\tau_G| \approx 0.12 \;\;\text{and}\;\; |\tau_K| \approx 0.255,\;\; |\tau_G| \approx 0.03, \tag{18.198}$$

respectively. The large size of $|\tau_K|$ reflects the bad quality of a mean-field description. The larger l gives the more physical estimate.

[1] L.D. Landau, J.E.T.P. *7*, 627 (1937); V.L. Ginzburg and L.D. Landau, J.E.T.P. *20*, 1064 (1950);

[2] V.L. Ginzburg, Fiz. Twerd. Tela **2**, 2031 (1960) [Sov. Phys. Solid State **2**, 1824 (1961)]. See also the detailed discussion in Chapter 13 of the textbook L.D. Landau and E.M. Lifshitz, *Statistical Physics*, 3rd edition, Pergamon Press, London, 1968.

[3] See Eq. (3.24) on p. 315 of the textbook in Footnote 3 where $g/a^3 \approx 111(T_c/T_F)^2$, with $T_F \approx 10^3T_c$.

[4] C.J. Lobb, Phys. Rev. B **36**, 3930 (1987).

[5] D.B. Murray and B.G. Nickel, (unpublished). R. Guida and J. Zinn-Justin, J. Phys. A **31**, 8130 (1998); H. Kleinert, FU-Berlin preprint 1999 (cond-mat/9906107).

[6] J.M. Kosterlitz and D.J. Thouless, J. Phys. C **6**, 1181 (1973), Prog. Low Temp. Phys. B **7**, 371 (1978).

[7] See Section 7.8. in the textbook in Footnote. 3.

[8] H. Kleinert and B. Van den Bossche, Phys. Lett. B **474**, 336 (2000) (hep-ph/9907274).

[9] See Fig. 5.3 on p. 428 in the textbook in Ref. 3.

[10] See pp. 256–257 in the textbook in Ref. 3.

19

Phase Transitions in Hydrodynamic Limit

So far we have seen two ways of describing phase transitions in an O(N)-symmetric system with th help of fluctuating fields. One used a ϕ^4-theory where a sign change of the mass term $m^2\phi^2$ caused a change of the potential from one with a unique minimum to one with a countinuous set of O(N)-symmetric degenerate minima, as illustrated in Fig. 15.1. The other was via a study of the Goldstone modes in the nonlinear σ-model, which are the modes moving only along the degenerate minima in the ϕ^4 potential. Here we were able to prove the existence of a phase transition only in the limit of large N.

If N is small, the nonlinear σ-model has to be studied by another technique, based on the statistical mechanics of topological defects. In an O(N)-model, these can be point-like, line-like, of surface-like. In such an approach the phase transition arises from the increasing significance of the configurational entropy with increasing temperature. Since the thermal generation of certain configurations is controlled by its free energy $F = E - TS$ of the system, defects whose energy E is much larger than the thermal energy k_BT can still be activated thermally at a moderate critical temperature $T_c = E/S$, if they exist in many possible configurations, i.e., with a large configurational entropy S. The problem of phase transitions is thereby reduced to a problem of *random geometries*.

Examles in nature are plentiful. In magnetic systems with an O(1)-symmetry (Ising systems), there are only two preferred directions, with domain walls separating them. The statistical mechanics of these domain walls can be idealized into a statistical mechanics of infinitely thin surfaces, and their proliferation at some temperature T_c determined by the balance of energy versus configurational entropy explains very well the Curie point. In O(2)-symmetric systems, most prominently superfluid helium, the transition to the normal phase can be described by the proliferation of vortex lines. In a crystal, the melting process is caused by a similar proliferation of defect lines.

In a magnet with O(3)-symmtry, as described by the classical Heisenberg model, the topological defects are hedgehog-like field configurations, and the study of a gas of these explains the demagnetization transition.

In this chapter we shall reformulate the functional integral of nonlinear σ-models in O(2)-symmetric systems in such a way that the topological defects are clearly exhibited, and appear in the partition function as s sum over all possible line configurations. This will enable us to find the temprature at which they proliferate.

An important tool for this study are disorder fields whose Feynman diagrams are direct pictures of the lines appearing in the partition functions.

hydrodynamic limit of the theory, defined at the end of Subsection 15.2.1. As in the nonlinear σ-model, we focus attention upon the Goldstone modes of the system.

19.1 Goldstone Modes with Line-like Topological Defects

The common property of the systems to be described in this chapter are the massless excitations caused by a spontanous breakdown of a continuous symmetry. These dominate their statistical properties at low temperatures.

In superfluid ^{4}He, the spontaneously broken symmetry is a $O(2)$ symmetry [recall the remark after Eq. (15.27)], where one usually replaces the two fields ϕ_1 and ϕ_2 by a complex order field $\phi(\mathbf{x}) \equiv \phi_1(\mathbf{x}) + \phi_2(\mathbf{x})$. Under the O(2) tranformation this picks up a phase factor

$$\phi(\mathbf{x}) \rightarrow e^{i\alpha}\phi(\mathbf{x}). \tag{19.1}$$

At low temperatures, the specific heat in superfluid helium is predominantly caused by the massless modes, which are called *second sound*. After quantization, these lead to the characteristic power behavior in the temperature

$$C \sim T^D, \tag{19.2}$$

in D space dimensions. The experimental curve in three-dimensional helium is shown in Fig. 19.1. For large temperatures, the specific heat flattens out and saturates at a value following the Dulong-Petit law which depends only on the number of harmonic degrees of freedom. At a temperature $T_c \approx 2.3$ K, there is a pronounced peak in the

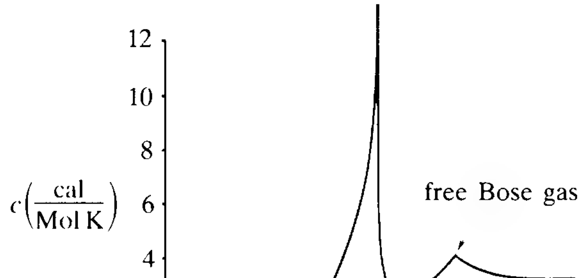

FIGURE 19.1 Specific heat of superfluid ^{4}He. The peak is caused by the superfluid-normal transition. A T^3-behavior is indicated as a dashed curve under the peak.

specifice heat which signalizes the second-order transition from the superfluid to the normal phase. This will be explained in this chapter from the statisticla properties of vortex lines.

In a crystal, the relevant massless modes are the quantized sound waves, the *phonons*. They are the Nambu-Goldstone modes of the spontanously broken translational invariance:

$$x_i \to x_i + \xi_i, \qquad \xi_i = \text{translation parameters}. \tag{19.3}$$

The sound waves are described by a *displacement field* $u_i(\mathbf{x})$ defined for each lattice point $\mathbf{x}$. The displacement field has a nontrivial topological property: It is only defined up to additional lattice vectors $\mathbf{a} \equiv (a_1, \dots, a_D)$. It is impossible to know whether a displaced atom at $x_i + u_i(\mathbf{x})$ has really come from $\mathbf{x}$, or from any other lattice point $\mathbf{x}'$. In a simple cubic crystal, the exponential field $\psi_i(\mathbf{x}) = e^{i2\pi u_i(\mathbf{x})/a}$ is is uniquely defined.

As in superfluid helium, the specific heat has, at low temperatures, the characteristic power behavior (19.209) as a function of temperature. As the temperature is raised, the T^D-behavior goes over into the typical Debye behavior. In crystals, it follows a universal function of T/Θ_D, where Θ_D is the Debye temperature. For $T > \Theta_D$, the specific heat flattens again out and saturates at a value following the Dulong-Petit law which depends only on the number of harmonic degrees of freedom. The experimental curve is shown in Fig. 19.2.

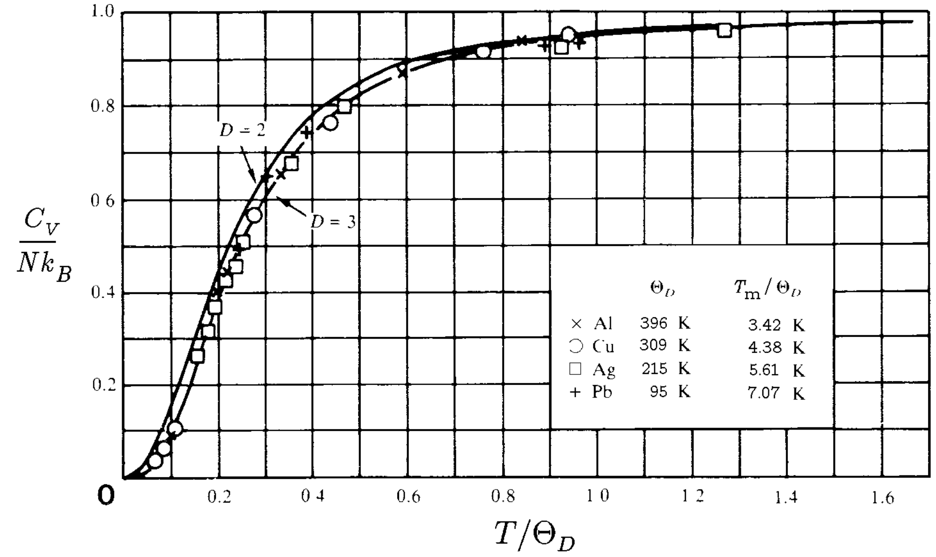

FIGURE 19.2 Specific heat of various solids. By plotting the data against the ratio T/Θ_D, where Θ_D is the Debye temperature, the data fall on a universal curve. The insert lists Θ_D-values and melting temperature $T_{\rm m}$.

In ferromagnets, it is the rotational symmetry of the direction $\mathbf{m}$ of the elementary magnets

$$\mathbf{m}(\mathbf{x}) \to R\,\mathbf{m}(\mathbf{x}), \qquad R = \text{arbitrary rotation matrix}, \tag{19.4}$$

which is spontaneously broken. The Nambu-Goldstone modes are magnons. As mentioned above, the topological defects are point-like hedgehog configurations. Their statistical mechanics will not be studied here.

The massless modes in superfluid helium and crystals are modified by anharmonic effects, which become visible at increasing temperatures and may be neglected in a qualitative discussion. In addition, there are usually massive excitations which, however, are strongly suppressed at low temperatures by a Boltzmann factor $y = e^{-E_{\rm a}/T}$ called the *fugacity* of the excitations. Here $E_{\rm a}$ is the *activation energy* defined as the energy of an excitation of infinite wave length, which in relativistic systems is called the *mass* of an excitation.

At a certain temperature T_c, which in solids lies above the Debye temperature, in quantum solids and superfluid ^{4}He near or below the Debye temperature, the statistical behavior undergoes a dramatic change. The physical properties of the system change in a phase transition. This often happens at energies where the fugacities of massive excitations are very small so that up to the transition, only Nambu-Goldstone modes should be substantially excited. The dramatic change is caused by the sudden appearance of line-like excitations, whose large activation energies are overcome by a high configurational entropy. In solids, these excitations are defect lines, in superfluids, they are vortex lines. This entropy mechanism was noted in the fifties by Shockley and Feynman. A line-like excitation of length l with an excitation energy ϵ per unit length is suppressed by a Boltzmann factor $e^{-\epsilon l/T}$. If the line can bend easily on a length scale ξ, it has roughly $(2D)^{l/\xi}$ possible configurations. We can therefore estimate the partition function of an ensemble of such lines with various length as

$$Z \approx \oint dl\,(2D)^{l/\xi} e^{-\epsilon l/T}. \tag{19.5}$$

The integral converges only below a critical temperature

$$T < T_c = \epsilon\xi/\log(2D). \tag{19.6}$$

Above T_c, the integral diverges and the ensemble undergoes a phase transition in which the lines proliferate and become infinitely long. We shall call this a *condensation process* of lines.

It is an interesting problem to construct a theory which explains such phase transitions with the help of these line-like excitations, without invoking explicitly the non-linear microscopic properties. This problem will be solve in the sequel. There exists a minimal extension of the Debye theory of the harmonic Nambu-Goldstone excitations which exhibit a phase transition caused by the condensation of idealized infinitely thin line-like excitations. The important theoretical tool to describe these is a new type of fluctuating fields which I call generically *defect gauge fields*, in the superfluid *vortex gauge fields*. In contrast to ordinary fluctuating fields, vortex or defect gauge fields have the useful property that they are capable of explaining the above phase transitions with a quadratic field action. This makes it easy to transform their partition functions to various other forms by quadratic manipulation of functional integrals. By a particular variable change, the partition function can be converted into an interacting field theory of the $|\phi|^4$-type which is called *disorder field theory*. We have observed this possiblity before when discussing Eq. (5.130), and at the end of Subsection 8.3.1.

The main difference with respect to the familiar order field theories of the Landau type is an opposite temperature behavior. In contrast to order fields, disorder fields acquire a nonzero expectation value at high temperatures.

In general, the line-like excitations are coupled to the Nambu-Goldstone modes. This gives rise to long-range interactions between the line elements. The interaction can be explained by a local field interaction if the description of the massless Nambu-Goldstone modes is changed into a gauge field description. This is always possible. The new gauge fields are called generically *stress gauge fields*. The associated gauge invariance is dual to that of the defect gauge fields.

In this way we arrive at a stress- and defect-gauge invariant theory of Goldstone modes and defect lines, or at an equivalent stress-gauge-invariant theory of disorder fields.

The appearance of topological defects has a simple general origin. Since Nambu-Goldstone modes occur as a result of a spontaneous breakdown of some continuous symmetry, their complex order field description has the form

$$\phi(\mathbf{x}) = e^{-i\theta_a(\mathbf{x})G^a}\phi_0 \tag{19.7}$$

where ϕ_0 is a fixed order parameter and G^a is a subset of generators of the associated symmetry group g. In the limit of infinite wave lengths, $\theta_a(\mathbf{x})$ becomes a constant and the energy is independent of θ_a— this being the reason for the masslessness the Nambu-Goldstone modes. In any order field theory of the Landau type, the so-called London limit selects from all excitations precisely the Nambu-Goldstone modes and approximates their field energy harmonically, while freezing all other excitations. The gradient energy of the order field gives rise to a euclidean action of the Nambu-Goldstone modes in the London limit

$$\mathcal{A}_{\rm NG} \propto \frac{1}{T}\int d^Dx|\boldsymbol{\nabla}e^{-i\theta_a(\mathbf{x})G^a}|^2. \tag{19.8}$$

It is a nontrivial to reexpress this action directly in terms of the $\theta_a(\mathbf{x})$-fields rather than the exponentials $e^{-i\theta_a(\mathbf{x})G^a}$. There always exist values of θ_a for which $e^{-i\theta_a)G^a}$ are identical. The field $\theta_a(\mathbf{x})$ can therefore jump between such values without any cost in gradient energy. If we want to describe the statistical mechanics of Nambu-Goldstone bosons, these jumps have to be included into the partition function. In systems with a spontanously broken O(2)-symmetry, this will be done with the help of vortex or defect gauge fields, as we are now going to explain by treating the several examples.

19.2 Superfluid ^{4}He

The simplest system containing Nambu-Goldstone modes is superfluid ^{4}He. They are describes by the phase factor of a complex order field

$$\phi(\mathbf{x}) = e^{i\theta(\mathbf{x})}\phi_0. \tag{19.9}$$

The line-like excitations are vortex lines.

19.2.1 Gradient Energy

In Landau's complex order field theory of superfluid ^{4}He, the invariance under $U(1)$ transformation

$$\phi(\mathbf{x}) \rightarrow e^{i\alpha}\phi(\mathbf{x}) \tag{19.10}$$

is spontaneously broken. As a consequence, the phase fluctuations of $\phi(\mathbf{x})$ are massless. On account of its exponential nature, the order field (19.9) has the following important topological property: For every point $\mathbf{x}$ it is possible to add an arbitrary integer-multiple of 2π without changing $e^{i\theta(\mathbf{x})}$. To formulate this properly, let us introduce a δ-function on a volume V:

$$\delta(\mathbf{x}; V) = \int d^3\bar{x}\delta^{(3)}(\mathbf{x} - \bar{\mathbf{x}}). \tag{19.11}$$

Then the above topological property of the order field amounts to an invariance under the replacement

$$\theta(\mathbf{x}) \rightarrow \theta(\mathbf{x}) + 2\pi\delta(\mathbf{x}; V). \tag{19.12}$$

The angular field $\theta(\mathbf{x})$ may jump by 2π across the surface S of an arbitrary volume V. When expressing the gradient energy (19.8) in terms of $\boldsymbol{\nabla}\theta$, this invariance must be maintained.

Moreover, the freedom of jumping by 2π across the surface of an arbitrary volumes V opens up the possibility of $\theta(\mathbf{x})$ jumping by 2π across an arbitrary open surface which does not enclose a volume but has a boundary line L. Due to the identity of the order field (19.9) on both sides, the jumping surface does not carry any energy. At the boundary L of the surface, however, the gradient energy $\boldsymbol{\nabla}e^{i\theta(\mathbf{x})}$ does not behave smoothly. The boundary line carries an energy. It is a *vortex line*. To describe the energy of such a configuration we define a δ-function on a surface in D dimensions

$$\delta_{ij}(\mathbf{x}; S) \equiv \int ds dt \left[\frac{\partial \bar{x}_j(s,t)}{\partial s}\frac{\partial \bar{x}_j(s,t)}{\partial t} - (st)\right]\delta^{(D)}(\mathbf{x} - \bar{\mathbf{x}}(s,t)). \tag{19.13}$$

In three dimensions, we form

$$\delta_k(\mathbf{x}; S) \equiv \frac{1}{2}\epsilon_{ijk}\delta_{jk}(\mathbf{x}; S). \tag{19.14}$$

It is now easy to see that the euclidean action associated with the correct gradient energy of the Nambu-Goldstone modes in the presence of a vortex line around S must read

$$\mathcal{A}_{\rm NG} = \frac{1}{2T}\int d^3x(\partial_i\theta - \theta_i^{\rm v})^2, \tag{19.15}$$

where

$$\theta_i^{\rm v}(\mathbf{x}) = 2\pi\delta_i(\mathbf{x};S) \tag{19.16}$$

removes the singularities in $\partial_i\theta(\mathbf{x})$ arising at the physically irrelevant jumps of the field $\theta(\mathbf{x})$.

Since the surface S is physically irrelevant, it can be deformed into any shape without changing the energy, as long as the boundary line stays the same. Indeed, under such a deformation $S \to S'$, the difference of the two surfaces encloses some volume V, and the δ-function (19.14) changes as follows:

$$\delta_i(\mathbf{x};S) \to \delta_i(\mathbf{x};S') = \delta_i(\mathbf{x};S) + \partial_i\delta(\mathbf{x};V). \tag{19.17}$$

For the field $\theta_i^{\rm v}(\mathbf{x})$, this implies

$$\theta_i^{\rm v}(\mathbf{x}) \to \theta_i^{\rm v}(\mathbf{x}) + \partial_i\Lambda_\delta(\mathbf{x}) \tag{19.18}$$

with the gauge function

$$\Lambda_\delta(\mathbf{x}) = 2\pi\delta(\mathbf{x};V). \tag{19.19}$$

The energy (19.15) is invariant under this, if $\theta(\mathbf{x})$ is simultaneously transformed as

$$\theta(\mathbf{x}) \to \theta(\mathbf{x}) + \Lambda_\delta(\mathbf{x}). \tag{19.20}$$

The field $\theta_i^{\rm v}$ is called the *vortex gauge field* of the superfluid and the combined transformation (19.18) and (19.20) is referred to as a *vortex gauge transformation.*

The subscript δ of the gauge function (19.19) emphasizes the fact that $\Lambda_\delta(\mathbf{x})$ is not an arbitrary function but a δ-functions on an arbitrary volume.

19.2.2 Vortex Density

The physical content of the vortex gauge field $\theta_i^{\rm v}(\mathbf{x})$ appears when forming its curl. By Stokes' theorem we find

$$\epsilon_{ijk}\partial_j\delta_k(\mathbf{x};S) = \delta_i(\mathbf{x};L) \tag{19.21}$$

where

$$\delta_i(\mathbf{x};L) = \int d\bar{x}_i\delta^{(3)}(\mathbf{x}-\bar{\mathbf{x}}) \tag{19.22}$$

is the δ-function on the boundary line L. The curl of $\theta_i^{\rm v}(\mathbf{x})$ is called the *vortex density*

$$\boldsymbol{\nabla}\times\boldsymbol{\theta}^{\rm v}(\mathbf{x}) = \mathbf{j}^{\rm v}(\mathbf{x}) = 2\pi\boldsymbol{\delta}(\mathbf{x};L) \tag{19.23}$$

As a consequence, the vortex density satisfies the obvious conservation law

$$\boldsymbol{\nabla}\cdot\mathbf{j}^{\rm v}(\mathbf{x}) = 0 \tag{19.24}$$

This states that vortex lines are closed.

The conservation law is a trivial consequence of $\mathbf{j}^{\mathrm{v}}$ being the curl of $\boldsymbol{\theta}^{\mathrm{v}}$. It is a Bianchi identity associated with the vortex gauge field structure.

The expression (19.15) may not yet be the complete energy of a vortex configuration. It is possible to add a gradient energy in the vortex gauge field. It introduces an extra *core energy* for the vortex line. The extended action is

$$\mathcal{A}_{\mathrm{NG}} = \int d^3x \left[\frac{1}{2T} (\boldsymbol{\nabla}\theta - \boldsymbol{\theta}^{\mathrm{v}})^2 + \frac{\epsilon_c}{2} (\boldsymbol{\nabla} \times \boldsymbol{\theta}^{\mathrm{v}})^2 \right]. \tag{19.25}$$

The core energy term is a square of a δ-function. It must be regularized by using a slightly smeared-out δ-functions over some small length scale a. This length scale will be set equal to unity in the entire lecture. The regularized last term is obviously proportional to the length of the lines.

19.2.3 Partition Function

The partition function Nambu-Goldstone modes and all possible vortex lines may be written as a functional integral

$$Z_{\mathrm{NG}} = \int \mathcal{D}\theta \sum_{\{S\}} e^{-\mathcal{A}_{\mathrm{NG}}}. \tag{19.26}$$

The measure $\int \mathcal{D}\theta$ is defined, as usual, by discretizing the space into a fine simple cubic lattice of spacing a and integration at each lattice point over all $\theta \in (-\infty, \infty)$, and taking the continuum limit $a \to 0$. The sum over all surface configurations is defined on the lattice by setting

$$\theta_i^{\mathrm{v}}(\mathbf{x}; S) \equiv 2\pi n_i(\mathbf{x}) \tag{19.27}$$

on each lattice point, where $n_i(\mathbf{x})$ is an integer-valued field, and by summing over all integer numbers $n_i(\mathbf{x})$

$$\sum_{\{S\}} = \sum_{\{n_i(\mathbf{x})\}} . \tag{19.28}$$

The partition function is then the continuum limit of the lattice approximation

$$\begin{aligned} Z_{\mathrm{latt}} &= \left[\prod_{\mathbf{x}} \int_{-\infty}^{\infty} d\theta(\mathbf{x}) \sum_{\{n_i(\mathbf{x})\}} \right] \\ &\quad \times e^{-\frac{1}{T}\int d^3x \left\{ \frac{1}{2}[\boldsymbol{\nabla}\theta(\mathbf{x}) - 2\pi \mathbf{n}(\mathbf{x})]^2 + \frac{\epsilon_c}{2}[\boldsymbol{\nabla}\times\mathbf{n}(\mathbf{x})]^2 \right\}}. \end{aligned} \tag{19.29}$$

which for $\epsilon_c = 0$ is the famous Villain approximation to the XY-model. The lattice spacing a has been set equal to unity and the symbol $\boldsymbol{\nabla}$ denotes the lattice derivative.

The vortex gauge fields requires a gauge fixing. On the lattice we can enforce the axial gauge

$$n_3(\mathbf{x}) = 0. \tag{19.30}$$

The Lorentz gauge $\boldsymbol{\nabla}\cdot\mathbf{n}=0$ cannot be chosen for integer-valued fields.

Similarly, the functional integral in the partition function (19.26) with the action (19.15) or (19.25) requires a gauge-fixing functional $\Phi[\boldsymbol{\theta}^{\rm v}]$, for which we choose the δ-functional

$$\Phi[\boldsymbol{\theta}^{\rm v}]=\delta[\theta_3^{\rm v}]. \tag{19.31}$$

Due to the sum over the vortex gauge fields $\boldsymbol{\theta}^{\rm v}$, the partition function (19.26) describes superfluid ^{4}He not only at zero temperature, where the Nambu-Goldstone modes were identified, but at any not too large temperature. In particular, the phase transition is *included*. The vortex gauge field enriches the ensemble of fluctuating Nambu-Goldstone modes in precisely the same way as the size of the order field ϕ does in a Landau description of the phase transition. In fact, it is easy to show that near the transition, the partition function (19.26) can be transformed into a $|\phi|^4$-theory of the Landau type.

19.2.4 Interaction Energy between Vortices

Let us calculate the interaction energy between vortex lines. Omitting the core energy, we expand the action (19.15) into

$$\mathcal{A}_{\rm NG}=\frac{1}{2T}\int d^3x\left[(\partial_i\theta)^2+2\theta\partial_i\theta_i^{\rm v}+\theta_i^{{\rm v}2}\right]. \tag{19.32}$$

A quadratic completion leads to

$$\mathcal{A}_{\rm NG}=\frac{1}{2T}\int d^3x\left\{\left[\partial_i\left(\theta+\frac{1}{-\boldsymbol{\nabla}^2}\boldsymbol{\nabla}\cdot\boldsymbol{\theta}^{\rm v}\right)\right]^2+\left(\boldsymbol{\theta}^{{\rm v}2}-\boldsymbol{\nabla}\cdot\boldsymbol{\theta}^{\rm v}\frac{1}{-\boldsymbol{\nabla}^2}\boldsymbol{\nabla}\cdot\boldsymbol{\theta}^{\rm v}\right)\right\} \tag{19.33}$$

In the partition function, the θ field can be integrated out producing a factor $\left[\mathrm{Det}(-\boldsymbol{\nabla}^2)\right]^{-1/2}$. The remaining action can be written as

$$\begin{aligned}\mathcal{A}_{\rm NG} &= \frac{1}{2T}\int d^3x(\boldsymbol{\nabla}\times\boldsymbol{\theta}^{\rm v})\frac{1}{-\boldsymbol{\nabla}^2}(\boldsymbol{\nabla}\times\boldsymbol{\theta}^{\rm v})\\ &= \frac{1}{2T}\int d^3x\,\mathbf{j}^{\rm v}\frac{1}{-\boldsymbol{\nabla}^2}\mathbf{j}^{\rm v}.\end{aligned} \tag{19.34}$$

This has the form of the magnetic Biot-Savart energy for current loops, except for an opposite sign (parallel currents attract each other, parallel vortices repel each other).

19.2.5 Kosterlitz-Thouless Transition in Films of Superfluid Helium

A thin layer of superfluid helim is called a film. If the thickness is smaller than the coherence length, such a film can be treated approximately like a two-dimensional system. In two dimensions, the vortex lines become vortex and antivortex pairs in the plane. We may imagine them as points of intercept of a closed vortex line with some plane, say the 1-2-plane, in a three-dimensional liquid. For a pair of these, , the vortex density is given by the third component , instead of (19.23), given by the throd component of

$$\boldsymbol{\nabla}\times\boldsymbol{\theta}^{\rm v}(\mathbf{x})=\mathbf{j}^{\rm v}(\mathbf{x})=2\pi\boldsymbol{\delta}(\mathbf{x};L),\tag{19.35}$$

which can be written more explicitly as

$$\left(\nabla_1\theta_2^{\rm v}-\nabla_2\theta_1^{\rm v}\right)(\mathbf{x})=j^{\rm v}(\mathbf{x})\equiv 2\pi[\delta(\mathbf{x}-\mathbf{x}_1),-\delta(\mathbf{x}-\mathbf{x}_2)],\tag{19.36}$$

where $\mathbf{x}_1$ and $\mathbf{x}_2$ are the positions of vortex and antivortex, respectively.

From what we have just learned, such a system has an interaction

$$\mathcal{A}_{\rm NG}\;=\;\frac{1}{2T}\int d^3x\,j^{\rm v}\frac{1}{-\boldsymbol{\nabla}^2}j^{\rm v}.\tag{19.37}$$

In coordinate space, the Coulomb propagator $-\boldsymbol{\nabla}^{-2}$ has been calculated in Eq. (17.94). It contains a small infrared cutoff mass μ and behaves in euclidean spacetime like

$$G(\mathbf{x}-\mathbf{x}')=-\frac{1}{2\pi}\log(\mu|\mathbf{x}-\mathbf{x}'|)+c,\qquad c=\frac{1}{2\pi}(\log 2-\gamma).\tag{19.38}$$

For a gas of vortices and antivortices at $\mathbf{x}_i$ $(i=1,2,3,\dots)$, we find from (19.37) a partition function

$$Z=\sum_{\text{all positions}}e^{-\mathcal{A}_{\rm NG}}=\sum_{\text{all positions}}\exp\left[-\frac{1}{2T}\sum_{i,j=1}q_iq_jG(\mathbf{x}_i-\mathbf{x}_j)\right],\tag{19.39}$$

where $q_i=2\pi$ for vortices and $q_i=-2\pi$ for antivortices. This partition function coincides with that of a gas of Coulomb particles with charges $\pm 2\pi$ in two dimensions.

The sum in the last exponent may be rewritten as follows:

$$\sum_{i,j=1}q_iq_jG(\mathbf{x}_i-\mathbf{x}_j)=\frac{1}{2T}\sum_{i,j=1}q_iq_j\left[G(\mathbf{x}_i-\mathbf{x}_j)-G(\mathbf{0})\right]+\left(\sum_i q_i\right)^2G(\mathbf{0}).\tag{19.40}$$

Now, $G(\mathbf{0})$ goes to plus infnity in the limit of zero infrared mass scale μ. This implies that the Boltzmann factors in (19.39) all vanish unless $\sum_i q_i=0$,i.e., unless the gas of vortices is neutral.neutrality condition For a neutral gas, the partition function becomes

$$Z=\sum_{\text{all positions}}\exp\left\{-\frac{1}{2T}\sum_{i,j=1}q_iq_j\left[G(\mathbf{x}_i-\mathbf{x}_j)-G(\mathbf{0})\right]\right\},\tag{19.41}$$

and the subtracted propagator was calculated in Eq. (17.97). It contains a large ultraviolet cutoff mass paramter Λ rather than the small infrared mass parameter μ. Inserting this into (19.2.5), we obtain

$$Z=\sum_{\text{all positions}}\exp\left\{\frac{1}{T}\sum_{i,j=1}q_iq_j\log(\Lambda|\mathbf{x}_i-\mathbf{x}_j|)\right\}=\sum_{\text{all positions}}\prod_{i,j=1}(\Lambda|\mathbf{x}_i-\mathbf{x}_j|)^{q_iq_j/4\pi T}.\tag{19.42}$$

The inverse ultraviolet cutoff $r_0 \equiv 1/\Lambda$ characterizes the size of the vortices, and may be identified with the coherence length in the superfluid film, usually of the order of 10 Å.

It is now easy to see that the partition function has a phase transition. In a very dilute system, we can focus attention on a single vortex-antivortex pair. Their average square distance is given by the expectation value of $r^2 \equiv |\mathbf{x}_1 - \mathbf{x}_2||^2$ within the partition function (19.2.5):

$$\langle r^2 \rangle = \int_{r_0}^{\infty} dr r \, r^2 e^{-(2\pi/T)\log(r/r_0)} \propto \frac{1}{2\pi/T - 4}. \tag{19.43}$$

This diverges as the reduced temperature increases above

$$T_{\rm KT} = \pi/2 \approx 1.5708. \tag{19.44}$$

The transition is a *vortex-antivortex separation transition*. It is of infinite order. A more detailed study shows that value (19.44) is an exact result for the transition temperature in a very dilute system of vortices and antivortices.[1]

19.2.6 Physical Jumping Surfaces

The gauge freedom in the partition function (19.26) is destroyed if the original $U(1)$ symmetry is explicitly broken. This adds a mass term to the Nambu-Goldstone modes, and the action (19.15) becomes

$$\mathcal{A}_{\rm NG} = \frac{1}{2T} \int d^3x \left\{ [\partial_i \theta(\mathbf{x}) - \theta^{\rm v}_i(\mathbf{x})]^2 + m^2 \theta(\mathbf{x})^2 \right\}. \tag{19.45}$$

As a consequence of the gauge dependence, the previously irrelevant surfaces become energetic. To see this we write the action as

$$\mathcal{A}_{\rm NG} = \frac{1}{2T} \int d^3x \left\{ \left[(\partial_i \theta)^2 + m^2 \theta^2 \right] - \theta \partial_i \theta^{\rm v}_i + \theta^{\rm v2}_i \right] \}. \tag{19.46}$$

Integrating out the θ-field in Z leads to an interaction

$$\mathcal{A}_{\rm int} = \frac{1}{2T} \int d^3x \left(\boldsymbol{\theta}^{\rm v2} - \boldsymbol{\nabla} \cdot \boldsymbol{\theta}^{\rm v} \frac{1}{-\boldsymbol{\nabla}^2 + m^2} \boldsymbol{\nabla} \cdot \boldsymbol{\theta}^{\rm v} \right). \tag{19.47}$$

This can be rewritten as

$$\mathcal{A}_{\rm int} = \frac{1}{2T} \int d^3 \left[(\boldsymbol{\nabla} \times \boldsymbol{\theta}^{\rm v}) \frac{1}{-\boldsymbol{\nabla}^2 + m^2} (\boldsymbol{\nabla} \times \boldsymbol{\theta}^{\rm v}) + m^2 \boldsymbol{\theta}^{\rm v} \frac{1}{-\boldsymbol{\nabla}^2 + m^2} \boldsymbol{\theta}^{\rm v} \right]. \tag{19.48}$$

The first term is of the Biot-Savart type: antiparallel line elements attract each other with a finite-range Yukawa potential $e^{-mr}/4\pi r$. The second term describes a Yukawa interaction between the normal vector of the surface elements. It produces a physical surface of thickness $1/m$.

The same gauge-breaking mechanism can be used to construct a simple model of quark confinement which will be described in Section 4.

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[1] See the textbook in Footnote 8.

19.2.7 Gauge Field of Superflow

There exists an alternative representation of the partition function in which the vortex lines appear directly via their physical vortex density; the jumping surfaces S being completely eliminated. This is possible by representing the Nambu-Goldstone modes in terms of a new gauge field. It is canonically conjugate to the angular field θ and called generically the *stress gauge field*, which here is the *gauge field of superflow*. Recall that the momentum variable in an ordinary path integral

$$\int \mathcal{D}x e^{-\int dt \dot{x}^2/2} \tag{19.49}$$

is introduced by a quadratic completion, rewriting (19.49) as

$$\int \mathcal{D}x\mathcal{D}p e^{\int dt\left(ip\dot{x}-\frac{p^2}{2}\right)}. \tag{19.50}$$

By analogy, we rewrite the partition function (19.26) as

$$Z = \int \mathcal{D}\theta \int \mathcal{D}b_i \sum_{\{S\}} e^{-\mathcal{A}^{\rm c}_{\rm NG}} \tag{19.51}$$

where[2]

$$\mathcal{A}^{\rm c}_{\rm NG} = \int d^3x \left\{ \frac{T}{2} b_i^2(\mathbf{x}) - ib_i \left[\partial_i \theta(\mathbf{x}) - \theta_i^{\rm v}(\mathbf{x})\right]\right\}. \tag{19.52}$$

Note that if we go over to a Minkowski space formulation in which $x^0 = -ix^3$ plays the role of the time, the integral

$$\int \mathcal{D}b_0 e^{-ib_0(\mathbf{x})\partial_0\theta} \tag{19.53}$$

creates on a discretized time axis a product of δ-functions

$$\langle\theta_{n+1}|\theta_n\rangle\langle\theta_n|\theta_{n-1}\rangle\langle\theta_{n-1}|\theta_{n-2}\rangle \tag{19.54}$$

with

$$\langle\theta_n|\theta_{n-1}\rangle = \delta_n(\theta_n - \theta_{n-1}) \tag{19.55}$$

which can be interpreted as Dirac scalar products in the Hilbert space of the system. On this Hilbert space, there exists an operator $\hat{b}_i(\mathbf{x})$ whose zeroth component is given by

$$\hat{b}_0 = -i\partial_\theta \tag{19.56}$$

and satisfies the equal-time canonical communication rule

$$\left[\hat{b}_0(\mathbf{x}_\perp, x_0), \theta(\mathbf{x}'_\perp, x_0)\right] = -i\delta^{(2)}(\mathbf{x}_\perp - \mathbf{x}'_\perp), \tag{19.57}$$

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[2] Similar canonical representations for the defect ensembles in a variety of physical systems are given in H. Kleinert, Phys. Lett. A **130** (1988). .

where $\mathbf{x}_\perp = (x^1, x^2)$ denotes the spatial components of the vector (x^0, x^1, x^2). The charge associated with $\hat{b}_0(\mathbf{x})$,

$$\hat{Q}(\mathbf{x}_0) = \int d^2x \hat{b}_0(\mathbf{x}_\perp, x_0), \tag{19.58}$$

generates a constant shift in θ:

$$e^{-i\alpha\hat{Q}(\mathbf{x}_0)}\theta(\mathbf{x}_\perp, x_0)e^{i\alpha\hat{Q}(\mathbf{x}_0)} = \theta(\mathbf{x}_\perp, x_0) + \alpha. \tag{19.59}$$

Thus it multiplies the original field $e^{i\theta(\mathbf{x})}$ by a phase factor $e^{i\alpha}$. The charge $\hat{Q}(\mathbf{x}_0)$ is the generator of the $U(1)$ symmetry transformation whose spontaneous symmetry breakdown is responsible for the Nambu-Goldstone nature of the phase fluctuations $\theta(\mathbf{x})$. Since the original theory is invariant under the transformations $\phi \to e^{i\alpha}\phi$, the energy (19.52) does not depend on θ itself, only on $\partial_i\theta$. Thus, in the partition function, the field θ can be integrated out using the formula

$$\int \mathcal{D}\theta e^{if(\mathbf{x})\theta} = \delta[f(\mathbf{x})]. \tag{19.60}$$

This produces the conservation law

$$\partial_i b_i(\mathbf{x}) = 0, \tag{19.61}$$

implying that $\hat{Q}(\mathbf{x}_0)$ is a time independent charge and $e^{i\alpha\hat{Q}}$ a symmetry transformation.

If the energy does depend on θ, the charge $\hat{Q}(\mathbf{x}_0)$ becomes x_0-dependent. However, it still generates the above $U(1)$ transformation.

The gradient energy could contain higher powers of $\partial_i\theta$. Then the canonical representation (19.52) contains more complicated functions of $b_i(\mathbf{x})$.

The conjugate variable to the phase angle of a complex field is the particle current, which is here the particle current in the superfluid condensate. Thus

$$j_i(\mathbf{x}) \equiv b_i(\mathbf{x}) \tag{19.62}$$

can be interpreted as the *supercurrent*.

The conservation law $\partial_i b_i(\mathbf{x}) = 0$ can be ensured automatically as a Bianchi identity, if we represent $b_i(\mathbf{x})$ as a curl of a gauge field of superflow

$$b_i(\mathbf{x}) = \epsilon_{ijk}\partial_j a_k(\mathbf{x}). \tag{19.63}$$

Then the action (19.52) goes over into

$$\mathcal{A}'^{\mathrm{c}}_{\mathrm{NG}} = \int d^3x \left[\frac{T}{2}(\boldsymbol{\nabla}\times\mathbf{a})^2 + i\mathbf{a}\cdot(\boldsymbol{\nabla}\times\boldsymbol{\theta}^{\mathrm{v}}) + \frac{\epsilon_c}{2T}(\boldsymbol{\nabla}\times\boldsymbol{\theta}^{\mathrm{v}})^2\right]. \tag{19.64}$$

The partition function becomes

$$Z = \int \mathcal{D}\mathbf{a} \sum_{\{S\}} e^{-\mathcal{A}^{\mathrm{c}}_{\mathrm{NG}}} \tag{19.65}$$

The action is doubly gauge invariant, under the gauge transformations of superflow

$$a_i(\mathbf{x}) \rightarrow a_i(\mathbf{x}) + \partial_i \Lambda^{\mathrm{s}}(\mathbf{x}), \tag{19.66}$$

and under the vortex gauge transformation (19.18) and (19.19):

$$\theta_i^{\mathrm{v}}(\mathbf{x}) \rightarrow \theta_i^{\mathrm{v}}(\mathbf{x}) + \partial_i \Lambda_\delta(\mathbf{x}), \tag{19.67}$$

with the gauge functions

$$\Lambda_\delta(\mathbf{x}) = 2\pi\delta(\mathbf{x}; V). \tag{19.68}$$

With respect to the first gauge structure, the current conservation law $\partial_i b_i(\mathbf{x})$ is a Bianchi identity.

The integrations in the partition function (19.65) require a gauge-fixing factor for both gauge fields. For the vortex gauge field, we use the axial factor (19.31), for the gauge field of superflow, any fixing will do, for instance the transverse one:

$$\Phi[\mathbf{a}] = \delta[\boldsymbol{\nabla} \cdot \mathbf{a}]. \tag{19.69}$$

The action $\mathcal{A}'^{\mathrm{c}}_{\mathrm{NG}}$ can also be written in short form as

$$\mathcal{A}'^{\mathrm{c}}_{\mathrm{NG}} = \int d^3x \left[\frac{T}{2}(\boldsymbol{\nabla} \times \mathbf{a})^2 + i\mathbf{a}\cdot\mathbf{j}^{\mathrm{v}} + \frac{\epsilon_c}{2T}\mathbf{j}^{\mathrm{v}2} \right]. \tag{19.70}$$

In this expression, the jumping surfaces have disappeared and the action depends only on the vortex lines. The partition function may be rewritten as

$$Z = \int \mathcal{D}\mathbf{a} \sum_{\{L\}} e^{-\mathcal{A}'^{\mathrm{c}}_{\mathrm{NG}}} \tag{19.71}$$

with a constraint

$$\Phi[\mathbf{j}^{\mathrm{v}}] = \delta[\boldsymbol{\nabla} \cdot \mathbf{j}^{\mathrm{v}}] \tag{19.72}$$

which ensures the closure of the vortex lines.

For a fixed set of lines L, the partition function (19.71) has a similar form as the magnetic partition function of a set of current lines. Around a vortex line, the field $\mathbf{b}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{a}(\mathbf{x})$ looks precisely like a magnetic field $\mathbf{B}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{x})$ around a current line. Thus, integrating out the vector potential $\mathbf{a}$ yields once more the same Biot-Savart interaction energies as obtained before in another way in Eq. (19.34).

Note that if the energy contains an explicit dependence like the mass term of the last section, there exists no $\mathbf{a}$-field representation of the Nambu-Goldstone modes.

19.2.8 Disorder Field Theory

The sum over all vortex line configurations in the partition function (19.71) can be done separately, defining an $\mathbf{a}$-dependent vortex partition function

$$Z^{\mathrm{v}}[\mathbf{a}] = \sum_{\{L\}} \delta[\boldsymbol{\nabla} \cdot \mathbf{j}^{\mathrm{v}}] \exp\left[-\int d^3x \left(\frac{\epsilon_c}{2T}\mathbf{j}^{\mathrm{v}2} + i\mathbf{a}\cdot\mathbf{j}^{\mathrm{v}} \right) \right]. \tag{19.73}$$

This can be viewed as a particular representation of an entirely different set of Nambu-Goldstone modes, the dual Nambu-Goldstone modes. To see this we make use of an important relation:

$$\sum_{\{\tilde{S}\}} e^{i\int d^3x \tilde{\boldsymbol{\theta}}^{\rm v}(\mathbf{x})\mathbf{f}(\mathbf{x})} = \sum_{\{L\}} \delta\left[\mathbf{f}(\mathbf{x}) - \boldsymbol{\delta}(L)\right]. \tag{19.74}$$

This can easily be proved by going on a lattice and using the Poisson formula

$$\sum_{n} e^{i2\pi n\mu} = \sum_{m} \delta(\mu - m). \tag{19.75}$$

It is therefore possible to rewrite the partition function (19.73) as follows

$$Z^{\rm v}[\mathbf{a}] = \sum_{\{\tilde{S}\}} \int \mathcal{D}j_i^{\rm v} \int \mathcal{D}\tilde{\theta} \exp\left\{-\int d^3x \left[\frac{\epsilon_c}{2T}\mathbf{j}^{{\rm v}2} + \frac{i}{2\pi}\mathbf{j}^{\rm v}\left(\boldsymbol{\nabla}\tilde{\theta} - \tilde{\boldsymbol{\theta}}^{\rm v}\right)\right]\right\}. \tag{19.76}$$

The $\tilde{\theta}$-integration produces the constraint (19.72) and ensures the closure of the vortex lines. Integrating out the $\mathbf{j}^{\rm v}$-field gives

$$Z^{\rm v}[\mathbf{a}] = \sum_{\{\tilde{L}\}} \int \mathcal{D}\tilde{\theta} \exp\left[-\frac{1}{8\pi^2}\frac{T}{\epsilon_c}\int d^3x (\partial_i\tilde{\theta} - \tilde{\theta}_i^{\rm v} - 2\pi a_i)^2\right]. \tag{19.77}$$

This is the Nambu-Goldstone theory of another $U(1)$-invariant $|\phi^4|$-theory, the above-mentioned disorder field theory. It differs from the initial $|\phi|^4$ theory by the presence of an external vortex gauge field $\mathbf{a}$ in the gradient term coupled via a covariant derivative. The disorder field partition function is

$$Z^{\rm v}[\mathbf{a}] = \int \mathcal{D}\phi\mathcal{D}\phi^* \exp\left\{-\int d^3x \left[|(\partial_i - 2\pi a_i)\varphi|^2 + m^2|\varphi|^2 + \frac{g}{4}|\varphi|^4\right]\right\}. \tag{19.78}$$

At high temperatures, the vortex lines in the disorder theory (19.77) described by $\tilde{\theta}_i^{\rm v}$ are frozen out. The functional integral over $\tilde{\theta}$ removes the longitudinal part of a_i, and we remain with

$$Z^{\rm v}[\mathbf{a}] = \exp\left(-T\frac{m_a^2}{2}\int d^3x\, \mathbf{a}_T^2\right) \tag{19.79}$$

where

$$m_a^2 = \frac{1}{\epsilon_c}, \tag{19.80}$$

and $\mathbf{a}_T$ is the transverse part of the the gauge field of superflow $\mathbf{a}$. It is defined by

$$a_{Ti} \equiv \left(\delta_{ij} - \partial_i\partial_j/\boldsymbol{\nabla}^2\right) a_j. \tag{19.81}$$

The exponent in (19.79) is a mass term for the transverse part of the gauge field.

In the complex disorder field theory (19.78), the mass term m^2 is negative and the disorder field acquires a nonzero expectation value $\phi_0 = \sqrt{-m^2/g}$. This produces again a mass term (19.79).

The mass term (19.79) shows that in the high-temperature phase, the singular nature of the vortex gauge field $\boldsymbol{\theta}^{\rm v}$ is lost and $\boldsymbol{\theta}^{\rm v}$ can be treated as an ordinary fluctuating transverse field. The sum $\sum_{\{\tilde{L}\}}$ turns into a functional integral over an ordinary gauge field $\int \mathcal{D}\boldsymbol{\theta}^{\rm v}$. Indeed, when doing this integral in the partition function out (19.73), we find that the vortex density has the simple correlation function

$$\langle j_i{}^{\rm v}(\mathbf{x}) j_j{}^{\rm v}(\mathbf{x}')\rangle = \frac{T}{\epsilon_c}(\delta_{ij} - \partial_i\partial_j/\boldsymbol{\nabla}^2)\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{19.82}$$

which produces directly the mass term (19.79).

This is to be contrasted with the contributions to the **a**-field action coming from $Z^v[\mathbf{a}]$ of Eq. (19.73) at low temperatures T. There the vortex lines form small loops, and these can be shown to give[3]

$$Z^{\rm v}[\mathbf{a}] \sim \exp\left[-\frac{1}{2}(\boldsymbol{\nabla}\times\mathbf{a})f(-i\boldsymbol{\nabla})(\boldsymbol{\nabla}\times\mathbf{a})\right], \tag{19.83}$$

where $f(-i\boldsymbol{\nabla})$ is some smooth function starting out with a constant, the so-called *stiffness* of the **a**-filed. The contributions of small vortex loops change only the dispersion of the gauge fields of superflow. Infinitely long vortex lines in $\boldsymbol{\theta}^{\rm v}$ are necessary to change the mass. These are present at high temperatures T where the correlation function of the vortex densities is (19.82).

With the help of the disorder partition function $Z^{\rm v}[\mathbf{a}]$, the partition function (19.26) of the Nambu-Goldstone modes associated with the action (19.25) can be replaced by another completely equivalent one:

$$\tilde{Z}_{\rm NG} = \int \mathcal{D}\mathbf{a} \sum_{\{\tilde{L}\}} \int \mathcal{D}\tilde{\theta}\, e^{-\tilde{\mathcal{A}}_{\rm NG}} \tag{19.84}$$

with the action

$$\tilde{\mathcal{A}}_{\rm NG} = T\int d^3x \left[\frac{1}{2}(\boldsymbol{\nabla}\times\mathbf{a})^2 + \frac{m_a^2}{8\pi^2}\left(\boldsymbol{\nabla}\tilde{\theta} - \tilde{\boldsymbol{\theta}}^{\rm v} - 2\pi\mathbf{a}\right)^2\right]. \tag{19.85}$$

This action is invariant under the following two types of gauge transformations. First, there is invariance under the gauge transformations of superflow (19.66), if it is accompanied by a compensating transformation of the angular field $\tilde{\theta}$:

$$a_i(\mathbf{x}) \to a_i(\mathbf{x}) + \partial_i\Lambda(\mathbf{x}), \qquad \tilde{\theta}(\mathbf{x}) \to \tilde{\theta}(\mathbf{x}) + 2\pi\Lambda(\mathbf{x}). \tag{19.86}$$

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[3] See the textbook in Footnote 19.4, Vol. I, Part 2, Sections 9.7 and 11.9, in particular Eq. (11.133); also H. Kleinert and W. Miller, Phys. Rev. Lett. **56**, 11 (1986); Phys. Rev. D **38**, 1239(1988).

Second, there is gauge invariance under the vortex gauge transformations of the disorder field, the analogs of Eqs. (19.18)–(19.20):

$$\tilde{\theta}^{\mathrm{v}}_i(\mathbf{x}) \to \tilde{\theta}^{\mathrm{v}}_i(\mathbf{x}) + \partial_i \tilde{\Lambda}_\delta(\mathbf{x}), \qquad \tilde{\theta}(\mathbf{x}) \to \tilde{\theta}(\mathbf{x}) + \tilde{\Lambda}_\delta(\mathbf{x}), \tag{19.87}$$

with gauge functions

$$\tilde{\Lambda}_\delta(\mathbf{x}) = 2\pi\delta(\mathbf{x}; \tilde{V}). \tag{19.88}$$

At high temperatures, the vortex lines in $\tilde{\boldsymbol{\theta}}^{\mathrm{v}}$ are frozen out and the action (19.85) shows again the mass term (19.79).

The mass term implies that at high temperatures, the gauge field of superflow possesses a finite range. At some critical temperature superfluidity has been destroyed. This is an analog of the Meissner effect within the disorder theory.[4] Note that in the absence of the gauge field of superflow $\mathbf{a}$, the field $\tilde{\theta}$ would be of long range, i.e., massless. The gauge field of superflow absorbs the massless mode and the system has only short-range excitations. More precisely, it can be shown that any correlation function involving local gauge-invariant observable quantities must be of short range in the high-temperature phase.

Take, for instance, the local gauge-invariant current operator of the disorder field

$$\mathbf{j}^s \equiv \boldsymbol{\nabla}\tilde{\theta} - \mathbf{a} \tag{19.89}$$

In the gauge $\tilde{\theta} \equiv 0$, we easily find

$$\langle j_i{}^s(\mathbf{x}_1) j_j{}^s(\mathbf{x}_2)\rangle \propto \int d^3k e^{i\mathbf{k}(\mathbf{x}_1-\mathbf{x}_2)} \frac{\delta_{ij} - k_i k_j/m_a^2}{\mathbf{k}^2 + m_a^2}. \tag{19.90}$$

This has *no* zero-mass pole.

19.2.9 Disorder Theory of Superconductor

A superconductor is described by the Ginzburg-Landau action

$$\mathcal{A}_{\mathrm{GL}} = \frac{1}{\tilde{T}} \int d^3x \left\{ |(\boldsymbol{\nabla} - i\mathbf{A})\varphi|^2 + m^2|\varphi|^2 + \frac{g}{2}|\varphi|^4 + \frac{1}{2}(\boldsymbol{\nabla}\times\mathbf{A})^2 \right\}. \tag{19.91}$$

We have set the charge of the Cooper pairs equal to unity, for simplicity. In the superconducting phase, m^2 is negative. ng to the *London limit*, the field φ is approximated by

$$\varphi = e^{i\theta(\mathbf{x})}\varphi_0 \tag{19.92}$$

with a constant real $\varphi_0 = \sqrt{-m^2/g}$, and the action becomes

$$\mathcal{A}_{\mathrm{LL}} = \frac{1}{\tilde{T}} \int d^3x \left[\frac{m_A^2}{2} \left(\boldsymbol{\nabla}\tilde{\theta} - \tilde{\boldsymbol{\theta}}^{\mathrm{v}} - \mathbf{A} \right)^2 + \frac{1}{2}(\boldsymbol{\nabla}\times\mathbf{A})^2 \right] \tag{19.93}$$

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[4] See H. Kleinert, Lett. Nuovo Cimento **35**, 405 (1982).

where we have set $\varphi_0^2 = m_A^2/2e^2$. The partition function reads

$$Z_{\rm SC} = \int \mathcal{D}\tilde\theta \int \mathcal{D}\mathbf{A} \sum_{\{\tilde L\}} e^{-\mathcal{A}_{\rm LL}}. \tag{19.94}$$

The action (19.93) has the same form as the action in the disorder representation (19.85) of superfluid ^{4}He. The role of the gauge field of superflow is now played by the vector potential **A** of magnetism. The action has the following two types of gauge invariances: the magnetic ones

$$A_i(\mathbf{x}) \rightarrow A_i(\mathbf{x}) + \partial_i\Lambda(\mathbf{x}), \qquad \tilde\theta(\mathbf{x}) \rightarrow \tilde\theta(\mathbf{x}) + \Lambda(\mathbf{x}), \tag{19.95}$$

and the vortex gauge transformations

$$\tilde\theta_i^{\rm v}(\mathbf{x}) \rightarrow \tilde\theta_i^{\rm v}(\mathbf{x}) + \partial_i\tilde\Lambda_\delta(\mathbf{x}), \qquad \tilde\theta(\mathbf{x}) \rightarrow \tilde\theta(\mathbf{x}) + \tilde\Lambda_\delta(\mathbf{x}), \tag{19.96}$$

with gauge functions

$$\tilde\Lambda_\delta(\mathbf{x}) = 2\pi\delta(\mathbf{x};\tilde V). \tag{19.97}$$

As in the description of superfluid ^{4}He by the partition function (19.26), the partition function (19.94) describes the statistical behavior of the superconductor not only at zero temperature, where the action (19.93) was constructed, but at all not too large temperatures. The fluctuating vortex gauge field $\tilde{\boldsymbol\theta}^{\rm v}$ ensures the validity through the phase transition.

We shall now derive the disorder representation of this partition function in which the vortex lines of the superconductor play a central role in describing the phase transition.

At low temperatures, the vortices are frozen, and the $\tilde\theta$-fluctuations in the partition function can be integrated out. This reduces the action to

$$\mathcal{A}_{\rm LL} \sim \frac{m_A^2}{2\tilde T}\int d^3x \mathbf{A}_T^2, \tag{19.98}$$

i.e., to a simple transverse mass term for the vector potential **A**. This is the famous Meissner effect in a superconductor, which limits the range of a magnetic field to a finite *penetration depth* $\lambda = 1/m_A$. The effect is completely analogous to the one observed previously in the disorder description of the superfluid where the superfluid acquired a finite range in the normal phase.

To derive the disorder theory of the partition function (19.94), we supplement the action by a core energy of the vortex lines

$$\mathcal{A}_{\rm core} = \frac{\tilde\epsilon_c}{2\tilde T}\int d^3x(\boldsymbol\nabla\times\tilde{\boldsymbol\theta}^{\rm v})^2. \tag{19.99}$$

As in the partition function (19.51), an auxiliary $\tilde b_i$ field can be introduced to bring the action (19.93) to the form

$$\tilde{\mathcal{A}}_{\rm LL} = \int d^3x \left[\frac{\tilde T}{2m_A^2}\tilde{\mathbf{b}}^2 + i\tilde{\mathbf{b}}\cdot\left(\boldsymbol\nabla\tilde\theta - \tilde{\boldsymbol\theta}^{\rm v} - \mathbf{A}\right) + \frac{1}{2\tilde T}\left(\boldsymbol\nabla\times\mathbf{A}\right)^2 + \frac{\tilde\epsilon_c}{2\tilde T}(\boldsymbol\nabla\times\tilde{\boldsymbol\theta}^{\rm v})^2\right]. \tag{19.100}$$

By integrating out the $\tilde{\theta}$-fields, we obtain the conservation law

$$\boldsymbol{\nabla}\cdot\tilde{\mathbf{b}}=0 \tag{19.101}$$

which we fulfill by introducing the gauge field of superflow in the superconductor

$$\tilde{\mathbf{b}}=\boldsymbol{\nabla}\times\tilde{\mathbf{a}}. \tag{19.102}$$

In this way, we find the action

$$\tilde{\mathcal{A}}_{\rm LL}=\int d^3x\left[\frac{\tilde{T}}{2m_A^2}(\boldsymbol{\nabla}\times\tilde{\mathbf{a}})^2-i\tilde{\mathbf{a}}\cdot(\boldsymbol{\nabla}\times\mathbf{A})+\frac{1}{2\tilde{T}}(\boldsymbol{\nabla}\times\mathbf{A})^2-i\tilde{\mathbf{a}}\cdot\tilde{\mathbf{j}}^{\rm v}+\frac{\tilde{\epsilon}_c}{2\tilde{T}}\tilde{\mathbf{j}}^{\rm v2}\right]. \tag{19.103}$$

where

$$\tilde{\mathbf{j}}^{\rm v}=\boldsymbol{\nabla}\times\tilde{\boldsymbol{\theta}}^{\rm v}. \tag{19.104}$$

At low temperatures $\tilde{T}$ where vortex lines are absent, the $\tilde{\mathbf{a}}$-field can be integrated out and yields once more the transverse mass term (19.98).

At high temperatures $\tilde{T}$, the vortex lines are prolific and the vector vortex gauge field $\tilde{\boldsymbol{\theta}}^{\rm v}$ can be integrated out like an ordinary field. With the help of the correlation function (19.82), we obtain the transverse mass term

$$\frac{\tilde{T}}{2m_A^2}\int d^3x\frac{m_a^2}{2}\tilde{\mathbf{a}}_T^2 \tag{19.105}$$

where

$$m_a^2=1/m_A^2\tilde{\epsilon}_c. \tag{19.106}$$

When integrating out the massive $\tilde{\mathbf{a}}$-field, no mass term is produced for the vector potential $\mathbf{A}$. Instead, the vector potential acquires the effective action

$$\mathcal{A}_{\mathbf{A}}=\frac{1}{2\tilde{T}}\int d^3x\ \boldsymbol{\nabla}\times\mathbf{A}\left(1+\frac{m_A^2}{-\boldsymbol{\nabla}^2+m_a^2}\right)\boldsymbol{\nabla}\times\mathbf{A}. \tag{19.107}$$

Expanding the denominator in powers of $-\boldsymbol{\nabla}^2$ we see that only gradient energies appear. Thus, apart from a modification of the dispersion, the vector potential is of long range giving Coulomb-like forces at large distances.

For the low-temperature mass value $m_a^2=0$, the second term reduces again a transverse mass term (19.98) associated with the Meissner effect.

We can represent the fluctuating vortices in the superconductor by a disorder field theory in the same way as we did for the vortices in the superfluid, i.e., we repeat the transformations from (19.73) to (19.77). The angular field variable of disorder will be called θ, the vortex lines in the disorder theory $\boldsymbol{\theta}^{\rm v}$. The disorder action reads

$$\tilde{\mathcal{A}}_{\rm LL}^{\rm D}=\int d^3x\Big[\frac{\tilde{T}}{2m_A^2}(\boldsymbol{\nabla}\times\tilde{\mathbf{a}})^2-i\tilde{\mathbf{a}}\cdot(\boldsymbol{\nabla}\times\mathbf{A})+\frac{1}{2\tilde{T}}(\boldsymbol{\nabla}\times\mathbf{A})^2 \\ +\frac{\tilde{T}}{8\pi^2m_A^2}m_a^2(\boldsymbol{\nabla}\theta-\boldsymbol{\theta}^{\rm v}-2\pi\tilde{\mathbf{a}})^2\Big]. \tag{19.108}$$

Near the phase transition, this is equivalent to a disorder field action

$$\tilde{\mathcal{A}}^{\rm D}_{\rm LL} \sim \int d^2x \Big[\frac{\tilde{T}}{2m_A^2} (\boldsymbol{\nabla}\times\tilde{\mathbf{a}})^2 - i\tilde{\mathbf{a}}\cdot(\boldsymbol{\nabla}\times\mathbf{A}) + \frac{1}{2\tilde{T}}(\boldsymbol{\nabla}\times\mathbf{A})^2 \\ + \left[(\boldsymbol{\nabla} - 2\pi\mathbf{a})\,\phi\right]^2 + m^2|\phi|^2 + \frac{g}{2}|\phi|^4 \Big]. \tag{19.109}$$

The loop diagrams of the disorder field ϕ are the pictures of the vortex lines.

Note that on the average, $i\tilde{\mathbf{a}}$ is equal to the magnetic field $\boldsymbol{\nabla}\times\mathbf{A}$.

The disorder field theory for the superconductor has recently led to a determination of the critical properties of the superconducting phase transition.[5] Within the Ginzburg-Landau theory, this is impossible since the renormalization group gives no infrared stable fixed point at all.

19.2.10 Order versus Disorder

Let us now study some basic features of ordered versus disordered phases.

Superfluid ^{4}He

The order parameter $\mathcal{O}$ of the original theory (19.15) or (19.25) is defined as the expectation value of the phase of the complex order field $O(\mathbf{x}) = e^{i\theta(\mathbf{x})}$:

$$\mathcal{O} \equiv \langle O(\mathbf{x})\rangle = \langle e^{i\theta(\mathbf{x})}\rangle. \tag{19.110}$$

Its behavior can best be studied by considering the correlation function of two order fields $O(\mathbf{x})$:

$$G_O(\mathbf{x},\mathbf{x}') = \langle e^{i\theta(\mathbf{x})} e^{-i\theta(\mathbf{x}')}\rangle. \tag{19.111}$$

In the low temperature phase, where vortices are rare the $\theta(\mathbf{x})$-field fluctuates almost harmonically. By Wick's theorem, we can then approximate

$$G_O(\mathbf{x}_1,\mathbf{x}_2) \approx e^{-\frac{1}{2}\langle[(\theta(\mathbf{x}_1)-\theta(\mathbf{x}_2)]^2\rangle}. \tag{19.112}$$

The correlation function of the $\theta(\mathbf{x})$-fields

$$\langle\theta(\mathbf{x}_1)\theta(\mathbf{x}_2)\rangle \approx T\int\frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{x}_1-\mathbf{x}_2)}\frac{1}{\mathbf{k}^2} = T\frac{1}{4\pi|\mathbf{x}_1-\mathbf{x}_2|} \tag{19.113}$$

goes to zero for $r \longrightarrow \infty$. After a renormalization of the fields, we see that

$$G_O(\mathbf{x}_1,\mathbf{x}_2) \xrightarrow[|\mathbf{x}_1-\mathbf{x}_2|\to\infty]{} \text{const.} \tag{19.114}$$

By the cluster property of correlation functions,

$$\langle O(\mathbf{x}_1)O(\mathbf{x}_2)\rangle \xrightarrow[|\mathbf{x}_1-\mathbf{x}_2|\to\infty]{} \langle O(\mathbf{x}_1)\rangle\langle O(\mathbf{x}_2)\rangle, \tag{19.115}$$

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[5] M. Kiometzis, H. Kleinert, and A.M.J. Schakel, Phys. Rev. Lett. **73**,,1975 (1994).

this implies that the order parameter is a constant:

$$\mathcal{O} = \langle O(\mathbf{x}) \rangle = \text{const.} \tag{19.116}$$

Let us calculate the order parameter in the high temperature phase. To find the correlation function $G_O(\mathbf{x}_1, \mathbf{x}_2)$, we insert into the partition function a term

$$e^{-iq(\mathbf{x})\theta(\mathbf{x})} \tag{19.117}$$

with two point sources of opposite charge at the points $\mathbf{x}_1$ and $\mathbf{x}_2$:

$$q(\mathbf{x}) = \delta^{(3)}(\mathbf{x} - \mathbf{x}_1) - \delta^{(3)}(\mathbf{x} - \mathbf{x}_2). \tag{19.118}$$

Considering the canonical representation (19.52) with an extra core energy of the vortex lines as in (19.25), we obtain an action

$$\mathcal{A} = \int d^3x \left[\frac{T}{2} b_i^2 - i b_i \left(\partial_i \theta - \theta_i^{\mathrm{v}} \right) + \frac{\epsilon_c}{2} (\boldsymbol{\nabla} \times \boldsymbol{\theta}^{\mathrm{v}})^2 + i q(\mathbf{x}) \theta(\mathbf{x}) \right]. \tag{19.119}$$

Integrating out the θ-field in the partition function gives the constraint

$$\partial_i b_i(\mathbf{x}) = -q(\mathbf{x}). \tag{19.120}$$

In the magnetic-field analogy, the point charges in $q(\mathbf{x})$ correspond to a magnetic monopole and an anti-monopole.

The constraint is solved by introducing a singular field

$$b_i^{\mathrm{m}}(\mathbf{x}) = -\delta_i(\mathbf{x}; \bar{L}) \tag{19.121}$$

where the line $\bar{L}$ runs from $\mathbf{x}_1$ to $\mathbf{x}_2$ along an arbitrary path. This field satisfies

$$\partial_i b_i^{\mathrm{m}}(\mathbf{x}) = -q(\mathbf{x}). \tag{19.122}$$

We can therefore write

$$\mathbf{b}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{a}(\mathbf{x}) - \mathbf{b}^{\mathrm{m}}(\mathbf{x}), \tag{19.123}$$

and the action (19.119) can be replaced by

$$\mathcal{A} = \int d^3x \left[\frac{T}{2} \left(\boldsymbol{\nabla} \times \mathbf{a} - \mathbf{b}^{\mathrm{m}} \right)^2 - i \mathbf{a} \cdot \mathbf{j}^{\mathrm{v}} + \frac{\epsilon_c}{2T} \mathbf{j}_c^{\mathrm{v}2} \right]. \tag{19.124}$$

The field $\mathbf{b}^{\mathrm{m}}(\mathbf{x})$ plays the role of a *monopole gauge field.*[6] Changing the line shape $\bar{L}$ at fixed ends results in a transformation

$$b_i^{\mathrm{m}}(\mathbf{x}) \to b_i^{\mathrm{m}}(\mathbf{x}) + \epsilon_{ijk} \partial_j \delta_k(\mathbf{x}; S), \tag{19.125}$$

where S is the surface over which the line $\bar{L}$ has swept. The action (19.124) remains invariant if the gauge field of superflow is simultaneously transformed as

$$a_i(\mathbf{x}) \to a_i(\mathbf{x}) + \delta_i(\mathbf{x}; S). \tag{19.126}$$

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[6] See textbook in Footnote 19.4, Vol. I, Part 2, Chapter 10.

The pure phase order field $e^{i\theta(\mathbf{x})}$ corresponds to a gauge field

$$b_i^{\rm m}(\mathbf{x}) = \delta_i(\mathbf{x};\bar{L}_1) \tag{19.127}$$

with a line $\bar{L}_1$ starting at $\mathbf{x}$ and running to infinity, i.e., it is represented in the functional integral for the partition function associated with the action (19.119) by the integrand

$$e^{i\theta(\mathbf{x})} \,\hat{=}\, e^{-T\int d^3x\left\{\frac{1}{2}\mathbf{b}^{\rm m}(\mathbf{x})^2-\mathbf{b}^{\rm m}(\mathbf{x})\cdot[\boldsymbol{\nabla}\times\mathbf{a}(\mathbf{x})]\right\}}. \tag{19.128}$$

When integrating out the gauge field of superflow $\mathbf{a}$ at low temperatures where the vortex lines are frozen out, the action the partition function contains $\mathbf{b}^{\rm m}$ in the form of a factor

$$e^{-\frac{T}{2}\int d^3x\left[\mathbf{b}^{{\rm m}\,2}-(\boldsymbol{\nabla}\times\mathbf{b}^{\rm m})\frac{1}{-\boldsymbol{\nabla}^2}(\boldsymbol{\nabla}\times\mathbf{b}^{\rm m})\right]} = e^{-\frac{T}{2}\int d^3x\,\boldsymbol{\nabla}\cdot\mathbf{b}^{\rm m}\frac{1}{-\boldsymbol{\nabla}^2}\boldsymbol{\nabla}\cdot\mathbf{b}^{\rm m}}. \tag{19.129}$$

From this we obtain the correlation function

$$G_O(\mathbf{x}_1,\mathbf{x}_2) = e^{-\frac{T}{2}\int d^3x q\frac{1}{-\boldsymbol{\nabla}^2}q}. \tag{19.130}$$

Inserting (19.122), this is precisely the correlation function (19.112) with (19.113), which goes to a constant for $|\mathbf{x}_1-\mathbf{x}_2'|\rightarrow\infty$ as in (19.114) implying a nonzero order parameter.

In the disorder version $\tilde{Z}_{\rm NG}$ of the partition function $Z_{\rm NG}$, it is easy to calculate the correlation function also in the high-temperature phase. There, the $\mathbf{a}$-field contains the transverse mass term (19.79) and the situation is very similar to that in Section 2.5. The line connecting the points $\mathbf{x}_1$ and $\mathbf{x}_2$ becomes physical and its energy grows linearly with the length of the line. Thus, the correlation function vanishes

$$G_O(\mathbf{x}_1,\mathbf{x}_2) \sim e^{-{\rm const}\cdot|\mathbf{x}_1-\mathbf{x}_2|} \xrightarrow[|\mathbf{x}_1-\mathbf{x}_2|\rightarrow\infty]{} 0. \tag{19.131}$$

By the cluster property (19.115) of correlation functions, this shows that the order parameter vanishes.

Note that precisely the same exponential falloff is found within Landau's complex order field theory:

$$\langle\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)\rangle \propto \int\frac{d^3k}{(2\pi)^3}e^{i\mathbf{k}(\mathbf{x}_1-\mathbf{x}_2)}\frac{1}{\mathbf{k}^2+m^2} = \frac{1}{4\pi}\frac{e^{-m|\mathbf{x}_1-\mathbf{x}_2|}}{|\mathbf{x}_1-\mathbf{x}_2|}. \tag{19.132}$$

The mechanism by which the finite range arises is, however, quite different. The size fluctuations of the order field play an essential role. In the partition function (19.26), their role is taken over by the fluctuations of the vortex gauge field $\boldsymbol{\theta}^{\rm v}$, as pointed out at the end of Section 2.3.

Superconductor

The order parameter of the superfluid supplies directly a disorder parameter of the superconductor. Inserting the monopole gauge field (19.127) into the actions (19.103), (19.108) and (19.108), we obtain the disorder field analogous to (19.128):

$$\tilde{D}(\mathbf{x}) \equiv e^{-\frac{1}{\tilde{T}}\int d^3x \left\{\frac{1}{2}\mathbf{b}^{\mathrm{m}}(\mathbf{x})^2 - \mathbf{b}^{\mathrm{m}}(\mathbf{x})\cdot[\boldsymbol{\nabla}\times\mathbf{A}(\mathbf{x})]\right\}}. \tag{19.133}$$

The action for the correlation function of a monopole antimonopole pair is

$$\mathcal{A} = \int d^3x \left[\frac{\tilde{T}}{2m_A^2}(\boldsymbol{\nabla}\times\tilde{\mathbf{a}})^2 - i\tilde{\mathbf{a}}\cdot(\boldsymbol{\nabla}\times\mathbf{A}) + \frac{1}{2\tilde{T}}(\boldsymbol{\nabla}\times\mathbf{A}-\mathbf{b}^{\mathrm{m}})^2 - i\mathbf{a}\cdot\tilde{\mathbf{j}}^{\mathrm{v}} + \frac{\tilde{\epsilon}_c}{2\tilde{T}}\tilde{\mathbf{j}}_c^{\mathrm{v}2}\right]. \tag{19.134}$$

with $\mathbf{b}^{\mathrm{m}}$ of Eq. (19.121). At low temperature $\tilde{T}$ of the superconductor, where the vortex lines of the superconductor are frozen out and the integral over the $\tilde{\mathbf{a}}$-field yields a mass term for the vector potential $\mathbf{A}$, this becomes

$$\mathcal{A} = \int d^3x \left\{\frac{1}{2\tilde{T}}\left[(\boldsymbol{\nabla}\times\mathbf{A}-\mathbf{b}^{\mathrm{m}})^2 + \frac{m_A^2}{2}\mathbf{A}_T^2\right] - i\mathbf{a}\cdot\tilde{\mathbf{j}}^{\mathrm{v}} + \frac{\tilde{\epsilon}_c}{2\tilde{T}}\tilde{\mathbf{j}}_c^{\mathrm{v}2}\right\}. \tag{19.135}$$

Just as in (19.131), the line connecting the endpoints acquires an energy and the correlation function has the property

$$G_{\tilde{D}}(\mathbf{x}_1,\mathbf{x}_2) \sim e^{-\mathrm{const}\cdot|\mathbf{x}_1-\mathbf{x}_2|} \xrightarrow[|\mathbf{x}_1-\mathbf{x}_2|\to\infty]{} 0, \tag{19.136}$$

implying a vanishing disorder parameter:

$$\tilde{\mathcal{D}} = \langle\tilde{D}(\mathbf{x})\rangle = 0. \tag{19.137}$$

In the normal phase of the superconductor, the monopole gauge field enters the action (19.107) which becomes

$$\mathcal{A}'_{\mathbf{A}} = \frac{1}{2\tilde{T}}\int d^3x\ (\boldsymbol{\nabla}\times\mathbf{A}-\mathbf{b}^{\mathrm{m}})\left(1+\frac{m_A^2}{-\boldsymbol{\nabla}^2+m_a^2}\right)(\boldsymbol{\nabla}\times\mathbf{A}-\mathbf{b}^{\mathrm{m}}). \tag{19.138}$$

As in (19.130), we obtain for a large distance between the monopole and the antimonopole a Coulomb interaction implying that the disorder parameter is a constant:

$$\tilde{\mathcal{D}} = \langle\tilde{D}(\mathbf{x})\rangle = \mathrm{const}. \tag{19.139}$$

It is worth pointing out that although there are no zero-mass excitations in a superconductor, there does exist a field which has long-range correlations in the superconductive phase. If there were no gauge field $\mathbf{A}$, the exponential field $e^{i\tilde{\theta}}$ would provide us with an order parameter (describing the condensate of Cooper pairs):

$$\tilde{\mathcal{O}} = \langle e^{i\tilde{\theta}}\rangle. \tag{19.140}$$

In the presence **A**, however, this is no longer true since $e^{i\tilde{\theta}}$ it is not gauge invariant. Its expectation value vanishes identically on account of Elitzur's theorem.[7] There exists, however, a simple gauge-invariant modification of this used first by Dirac.[8] Let

$$Q(\mathbf{x}') \equiv \delta^{(3)}(\mathbf{x}' - \mathbf{x}) \tag{19.141}$$

be a charge density localized at the point **x**. Then the disorder field

$$\tilde{O}(\mathbf{x}) \equiv e_{\rm gi}^{i\tilde{\theta}(\mathbf{x})} \equiv \exp\left[i\int d^3x \left(\tilde{\theta} + \frac{\mathbf{A}\cdot\boldsymbol{\nabla}}{\boldsymbol{\nabla}^2}\right)Q\right] \tag{19.142}$$

is gauge invariant and the expectation value

$$\tilde{\mathcal{O}} = \langle e_{\rm gi}^{i\tilde{\theta}(\mathbf{x})}\rangle \tag{19.143}$$

is nonzero.

Note that apart from being invariant under magnetic gauge transformations

$$A_i(\mathbf{x}) \to A_i(\mathbf{x}) + \partial_i\Lambda(\mathbf{x}), \tag{19.144}$$

the disorder field (19.142) is trivially invariant under the vortex gauge transformations (19.87).

At low temperatures where the vortex lines can be ignored, it can easily be shown to be nonzero. We calculate the Green function associated with two fields (19.142):

$$G_{\tilde{O}}(\mathbf{x}_1, \mathbf{x}_2) \equiv \langle e_{\rm gi}^{i\tilde{\theta}(\mathbf{x}_1)} e_{\rm gi}^{-i\tilde{\theta}(\mathbf{x}_2)}\rangle. \tag{19.145}$$

In the transverse gauge, we can easily integrate out the $\tilde{\theta}$-fluctuations in (19.84) and find the same correlation function as in (19.114):

$$G_{\tilde{O}}(\mathbf{x}_1, \mathbf{x}_2) \xrightarrow[|\mathbf{x}_1-\mathbf{x}_2|\to\infty]{} \text{const.} \tag{19.146}$$

Hence

$$\tilde{\mathcal{O}} = \langle e^{\tilde{\theta}(\mathbf{x})_{\rm gi}}\rangle = \text{const.} \tag{19.147}$$

This is nonzero, just as the order parameter of the superfluid in the low temperature phase.

The reason why $e_{\rm gi}^{i\tilde{\theta}(\mathbf{x})}$ can have long-range correlations in spite of the absence of massless excitations is the nonlocal nature of this order field. All physical excitations are carries by gauge-invariant *local* fields which have short-range correlations.

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[7] S. Elitzur, Phys. Rev. D **12**, 3978 (1975).

[8] P.A.M. Dirac, *Principles of Quantum Mechanics*, 4th ed., Clarendon, Cambridge 1981, Section 80. J. Schwinger, Phys. Rev. *115*, 721 (1959); *127*, 324 (1962).

19.2.11 Order of Superconducting Phase Transition and Tricritical Point

In the superconducting phase, there are only a few vortex lines and the field ϕ fluctuates around zero. The mass term is $m^2 > 0$. The vector potential $\mathbf{A}$ may be integrated out and leads to an action for the $\mathbf{a}$-field

$$\mathcal{A}_{\mathbf{a}} = \int d^3x \left[\frac{1}{2m_A^2} (\boldsymbol{\nabla} \times \mathbf{a})^2 + \frac{1}{2} \mathbf{a}_T^2 + \mathbf{a}_T^2 \frac{c}{2} |\phi|^2 \right] \tag{19.148}$$

with some constant c. We have chosen a gauge where ϕ is real to make the coupling between $\mathbf{a}$ and ϕ simple. This yields also a coupling term $\mathbf{a}_L^2 |\phi|^2$ involving the longitudinal components of the field $\mathbf{a}$. When integrating out the longitudinal part, the functional determinant is canceled by the gauge-fixing factor of the gauge ϕ=real.

The $\mathbf{a}$-field can now be integrated out; for a constant ϕ, this yields an effective action

$$\mathcal{A} = \frac{1}{2} \mathrm{Tr} \log \left(-\boldsymbol{\nabla}^2 + m_A^2 + m_A^2 c |\phi|^2 \right). \tag{19.149}$$

When expanded in powers of $|\phi|^2$, this produces a term

$$- c^2 m_A^4 \int d^3x \int \frac{d^3k}{(2\pi)^3} \frac{1}{(k^2 + m_A^2)^2} |\phi|^4 \propto -m_A^3 \int d^3x |\phi|^4. \tag{19.150}$$

This term lowers the $(g/4)|\phi|^4$ interaction term in (19.109) . An increase in m_A corresponds to a decrease of the penetration depth in the superconductor, i.e. to materials moving towards the type-I regime. At some larger value of m_A, the $|\phi|^6$-term vanishes and the disorder field theory requires a $|\phi|^4$-term to stabilize the fluctuations of the vortex lines. In such materials, the superconducting phase transition turns from second to first order. The existence and position of such a tricritical point was first established on theoretical grounds in 1982.[9]

19.2.12 Vortex Lattices

The model action (19.15) represents the gradient energy in superfluid ^{4}He correctly only in the long-wavelength limit. The neutron scattering data yield the energy spectrum $\omega = \epsilon(\mathbf{k})$ shown in Fig. 19.3. To account for this, the action should be taken as follows:

$$\mathcal{A}_{\mathrm{NG}} = \frac{1}{2T} \int d^3x (\boldsymbol{\nabla}\, \theta - \boldsymbol{\theta}^{\mathrm{v}}) \frac{\epsilon^2(-i\boldsymbol{\nabla})}{-\boldsymbol{\nabla}^2} (\boldsymbol{\nabla}\, \theta - \boldsymbol{\theta}^{\mathrm{v}}). \tag{19.151}$$

The *roton peak* near 2Å^{-1} gives rise to a repulsion between opposite vortex line elements at the corresponding distance. If a layer of superfluid ^{4}He is diluted with

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[9] See the reference in Footnote 4 and the detailed discussion in the textbook quoted in Fottnote 19.4, Vol I, Part 2, Section 13, where the final disorder theory was derived [see, in particular, Eq. (13.30)].

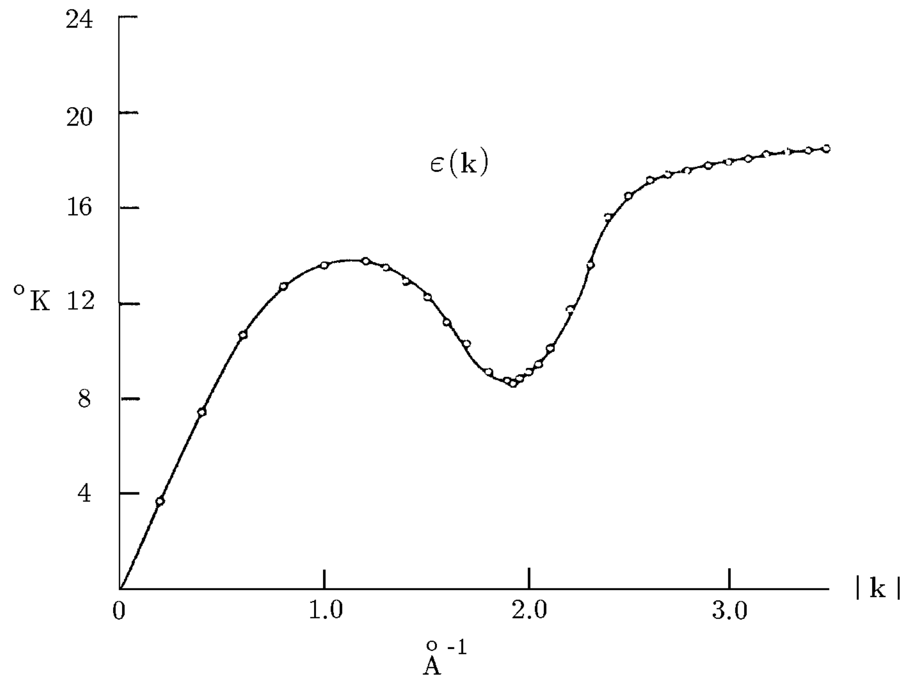

FIGURE 19.3 Energies of the elementary excitations of superfluid ^{4}He measured by neutron scattering, showing the excitation energy of the Nambu-Goldstone bosons [after R.A. Cowley and A.D. Woods, Can. J. Phys **49**, 177 (1971).

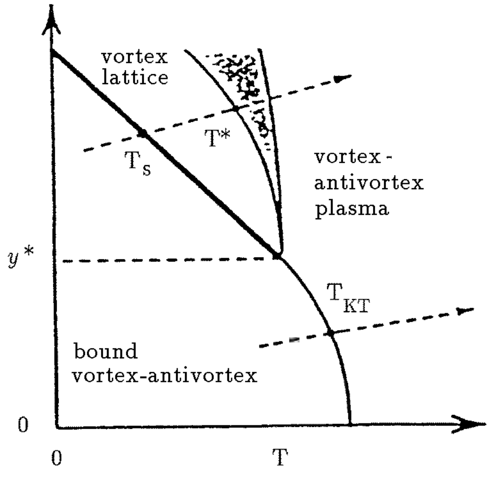
vortex lattice
T*
T_s
vortex - antivortex plasma
y^*
T_{KT}
bound vortex-antivortex
0
0
T

FIGURE 19.4 Phase diagram of a two-dimensional layer of superfluid ^{4}He. At a higher fugacity $y > y^*$, an increase in temperature causes the vortices to first condense to a lattice and to undergo a Kosterlitz-Thouless vortex unbinding transition only after a melting transition.

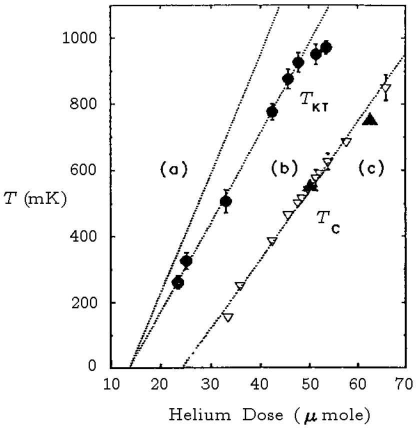

FIGURE 19.5 Experimental phase diagram of a two-dimensional layer of superfluid ^{4}He diluted with ^{3}He which decreases the fugacity and separates the vortex melting transition from the Kosterlitz-Thouless transition.

^{3}He, the core energy of the vortices decreases, the fugacity y and the average vortex number increases. For a sufficiently high average spacing, a vortex lattice forms. In this regime, the superfluid has three transitions when passing from zero temperature to the normal phase. There is first a condensation process to a vortex lattice, then a melting transition of this lattice into a fluid of bound vortex-antivortex pairs, and finally a pair-unbinding transitions of the Kosterlitz-Thouless type.[10] The latter two transitions have been seen experimentally.[11]

19.3 Crystals

In crystals, the elastic energy is usually expressed in terms of a material *displacement field* $u_i(\mathbf{x})$ as

$$E = \int d^3x u_{ij}^2(\mathbf{x}) \tag{19.152}$$

where

$$u_{ij}(\mathbf{x}) = \frac{1}{2}[\partial_i u_j(\mathbf{x}) + \partial_j u_j(\mathbf{x})] \tag{19.153}$$

is the *strain tensor*. For simplicity, we have set the shear elastic constant μ equal to unity and neglected the second elastic term $\lambda(\partial_i u_i)^2$. The elastic energy goes to zero for infinite wave length since in this limit $u_i(\mathbf{x})$ reduces to a pure translation and the energy of the system is translationally invariant. The crystallization process causes a spontaneous breakdown of the translational symmetry of the system. The elastic distortions describe the Nambu-Goldstone modes resulting from this symmetry breakdown.

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[10] M. Gabay and A. Kapitulnik, Phys. Rev. Lett. *71*, 2138 (1993); S.-C. Zhang, ibid., 2142 (1993).

[11] M.T. Chen, J.M. Roessler, and J.M. Mochel, J. Low Temp. Phys. *89*, 125 (1992).

A crystalline material always contains defects. In their presence, the elastic energy is

$$E=\int d^3x(u_{ij}-u^{\rm p}_{ij})^2 \tag{19.154}$$

where $u^{\rm p}_{ij}$ is the so-called *plastic strain tensor* describing the defects. Topologically, the crystal defects arise as a consequence of the multivaluedness of the displacement field on a lattice. Due to the identity of the lattice constituents, the displacement is defined only modulo lattice vectors. For mathematical simplicity, let us assume the lattice to be simple cubic of spacing 2π. Then the energy of $u_i(\mathbf{x})$ and $u_i(\mathbf{x})+2\pi N_i(\mathbf{x})$ must be indistinguishable for integer valued fields $N_i(\mathbf{x})$ which correspond to a permutation of the lattice sites. The order field of a crystal has therefore the three components

$$\phi_i(\mathbf{x})=e^{i2\pi u_i(\mathbf{X})}\phi_{0i}. \tag{19.155}$$

This is very similar to the order field of a superfluid. There are now three types of surfaces where the *distortion tensor* $\beta_{il}\equiv\partial_i u_l$ jumps by 2π, one for every lattice direction $b_l=1,2,3$. They are describes by the *plastic distortion*

$$\beta^{\rm p}_{il}(\mathbf{x})=\delta_i(\mathbf{x};S)b_l. \tag{19.156}$$

The surfaces S are irrelevant and correspond to a layer of atoms missing from a crystal. Only the boundary line is physical. They are called *dislocation lines* of Burgers vector b_l. The irrelevant surfaces S are called *Volterra surfaces* of the dislocation lines. The dislocation lines are extracted from $\beta^{\rm p}_{ij}$ by forming the dislocation density

$$\alpha_{il}(\mathbf{x})=\epsilon_{imn}\partial_m\beta^{\rm p}_{nl}(\mathbf{x})=\delta_i(L)b_l. \tag{19.157}$$

Being a curl, it satisfies the conservation law

$$\partial_i\alpha_{il}=0 \tag{19.158}$$

trivially as a Bianchi identity. The conservation law states that dislocation lines are closed.

A closed Volterra surface is associated with a translation

$$u_i(\mathbf{x})\rightarrow u_i(\mathbf{x})+2\pi b_i\delta(\mathbf{x};V) \tag{19.159}$$

where V is the volume enclosed by the closed Volterra surface S. Under such an operation, the order parameters $e^{iu_i(\mathbf{x})}$ are invariant.

In a real crystal, dislocation lines are able to stack up on top of each other forming line-like defects called *disclination lines*. Their geometric properties are most easily understood by noting that instead of the trivial translation (19.159) across a closed Volterra surface we can form a combined translation rotation plus

$$u_i(\mathbf{x})\rightarrow\left[b_i+R_{ij}u_j(\mathbf{x})\right]\delta(\mathbf{x};V) \tag{19.160}$$

where R_{ij} is a discrete rotation under which the crystal is invariant (in a simple cubic lattice, R_{ij} consists of products of rotations by $\pi/2$). The nonabelian nature of the trivial gauge transformations (19.160) makes a full discussion of the plastic deformations quite complicated. A useful approximation consists in assuming R_{ij} to be a small rotation and to reexpress (19.160) in the infinitesimal form

$$u_l(\mathbf{x}) \to u_l(\mathbf{x}) + (b_l + \epsilon_{lqr}\Omega_q x_r)\delta(\mathbf{x};V). \tag{19.161}$$

Assuming the presence of a closed Volterra surface, we extract the jumps in the distortion field

$$\beta_{kl} \equiv i\partial_k u_l(\mathbf{x}) = \delta_k(\mathbf{x};S)(b_l + \epsilon_{lqr}\Omega_q x_r) - \delta(\mathbf{x};V)\epsilon_{lqk}\Omega_q. \tag{19.162}$$

The first term is defined also for an open surface in which case it becomes the plastic distortion of a general defect line

$$\beta^{\mathrm{P}}_{kl} = \delta_k(\mathbf{x};S)(b_l + \epsilon_{lpr}\Omega_q x_r). \tag{19.163}$$

By forming the curl of the distortion field (19.162), the term $\delta(\mathbf{x};V)$ drops out and we find

$$\alpha_{il} = \epsilon_{ijk}\partial_j\partial_k u_l(\mathbf{x}) = \delta_i(\mathbf{x};L)(b_l + \epsilon_{lqr}\Omega_q x_r). \tag{19.164}$$

This is called the *dislocation density* of the defect line. The rotation field

$$\omega_j = \frac{1}{2}\epsilon_{jkl}\partial_k u_l \tag{19.165}$$

has the following derivative

$$\partial_n\omega_j = \frac{1}{2}\epsilon_{jkl}\partial_k\partial_n u_l = \frac{1}{2}\epsilon_{jkl}\partial_k\beta^{\mathrm{P}}_{nl} + \delta_n(\mathbf{x};S)\Omega_j. \tag{19.166}$$

The last term (19.166) is called the *plastic rotation*

$$\phi^{\mathrm{P}}_{nj} = \delta_n(s)\Omega_j. \tag{19.167}$$

The entire tensor (19.166) is called the *plastic bend-twist*

$$\kappa^{\mathrm{P}}_{nj} \equiv \partial_n\omega_j = \frac{1}{2}\epsilon_{jkl}\partial_n\beta^{\mathrm{P}}_{kl} + \phi^{\mathrm{P}}_{nj}. \tag{19.168}$$

The curl of the plastic rotation is the *disclination density*

$$\theta_{il} = \epsilon_{ijk}\partial_j\phi^{\mathrm{P}}_{kl} = \delta_i(\mathbf{x};L)\Omega_l. \tag{19.169}$$

Being a curl, this satisfies the conservation law

$$\partial_i\theta_{il} = 0 \tag{19.170}$$

implying that disclination lines are closed. This is again a Bianchi identity of the defect system. The conservation law for dislocations is modified by the presence of disclination as follows:

$$\partial_i\alpha_{ik} = -\epsilon_{kmn}\theta_{mn}. \tag{19.171}$$

Dislocation lines can now end in disclination lines.

An important geometric quantity characterizing dislocation and disclination lines is the *incompatibility* or *defect density*

$$\eta_{ij}(\mathbf{x}) = \epsilon_{ikl}\epsilon_{jmn}\partial_k\partial_m u_{ln}(\mathbf{x}). \tag{19.172}$$

It can be decomposed into disclination and dislocation density as follows:

$$\eta_{ij}(\mathbf{x}) = \theta_{ij}(\mathbf{x}) + \frac{1}{2}\partial_m\left[\epsilon_{min}\alpha_{jn}(\mathbf{x}) + (i \leftrightarrow j) - \epsilon_{ijn}\alpha_{mn}(\mathbf{x})\right]. \tag{19.173}$$

This tensor is symmetric and conserved

$$\partial_i\eta_{ij}(\mathbf{x}) = 0, \tag{19.174}$$

again a Bianchi identity of the defect system.

The tensors α_{ij}, θ_{ij} and η_{ij} are linearized versions of important tensors in a *Riemann-Cartan space* , a noneuclidean space with curvature and torsion. Such a space can be generated from a flat space by a plastic distortion, which is mathematically represented by a *nonholonomic* mapping

$$x_i \to x_i + u_i(\mathbf{x}). \tag{19.175}$$

Such a mapping is nonintegrable. The displacement fields and their first derivatives fail to satisfy the Schwarz integrability criterion:

$$\begin{aligned} \left(\partial_i\partial_j - \partial_j\partial_i\right) u(\mathbf{x}) &\neq 0 \\ \left(\partial_i\partial_j - \partial_j\partial_i\right) \partial_k u_l(\mathbf{x}) &\neq 0. \end{aligned} \tag{19.176}$$

The affine connection of the geometry in the plastically distorted space is

$$\Gamma_{ijl} = \partial_i\partial_j u_l. \tag{19.177}$$

The noncommutativity of the derivatives in front of $u_l(\mathbf{x})$ implies a nonzero torsion, the torsion tensor being

$$S_{ijk} \equiv (\Gamma_{ijk} - \Gamma_{jik})/2. \tag{19.178}$$

The dislocation density α_{ij} is equal to

$$\alpha_{ij} = \epsilon_{ikl}S_{klj}, \tag{19.179}$$

The noncommutativity of the derivatives in front of $\partial_k u_l(\mathbf{x})$ implies a nonzero curvature. The disclination density θ_{ij} is the Einstein tensor

$$\theta_{ij} = G_{ij} \equiv R_{ji} - \frac{1}{2}g_{ji}R \tag{19.180}$$

of this geometry. The tensor η_{ij}, finally, is the Belinfante symmetric energy momentum tensor which coincides with the Einstein tensor obtained from the Christoffel symbols of the metric

$$g_{ij} = \delta_{ij} + \partial_i u_j + \partial_j u_i \tag{19.181}$$

rather than from the affine connection Γ_{ijk}. To verify this statement we just note that the spin current density of the gravitational field is (setting the gravitational constant equal to unity)

$$\Sigma_{ij,k} = -2\left(S_{ijk} + \delta_{ik}S_j - \delta_{jk}S_i\right). \tag{19.182}$$

For more details on the geometric aspects see Vol. II of textbook in Footnote 19.4, Part IV, where the full one-to-one correspondence between defect systems and Riemann-Cartan geometry is developed as well as a gravitational theory based on this analogy.

It is possible to write down an elastic energy which disentangles dislocations and disclinations by including higher gradients of the displacements field. This energy reads

$$E = \int d^3x \left[\left(u_{ij} - u^{\rm p}_{ij}\right)^2 + \ell^2\left(\partial_i\omega_j - \kappa^{\rm p}_{ij}\right)^2\right]. \tag{19.183}$$

The parameter ℓ is the length scale over which the crystal is rotationally stiff.

The partition function contains integrals over u_i and sums over the jumping surfaces of dislocations and disclinations. By integrating out the u_i-fields, one obtains a Biot-Savart type of interaction energy between the defect lines in which dislocation line elements interact with each other via a Coulomb potential, whereas disclination line elements interact via a linearly rising potential.

It is again possible to eliminate the jumping surfaces from the partition function by introducing conjugate variables and associated stress gauge fields. For this we rewrite the elastic action of defect lines as

$$E = \int d^3x \left[\frac{1}{4T}\left(\sigma_{ij} + \sigma_{ji}\right)^2 + \frac{1}{8\ell^2}\tau_{ij}^2 + i\sigma_{ij}\left(\partial_i u_j - \epsilon_{ijk}\omega_k - \beta^{\rm p}_{ij}\right) + i\tau_{ij}\left(\partial_i\omega_j - \phi^{\rm p}_{ij}\right)\right], \tag{19.184}$$

and form the partition function by integrating over $\sigma_{ij}, \tau_{ij}, u_i, \omega_j$ and summing over all jumping surfaces S in the plastic fields. A functional integral over the antisymmetric part of σ_{ij} has been introduce the obtain an independent integral over ω_i [if we were to integrate out the antisymmetric part of σ_{ij}, we would enforce the relation $\omega_i = \frac{1}{2}\epsilon_{ijk}(\partial_j u_k + \beta^{\rm p}_{ij})$]. By integrating out ω_j and u_i, we find the conservation laws

$$\partial_i\sigma_{ij} = -\epsilon_{jkl}\tau_{kl}, \qquad \partial_i\tau_{ij} = 0. \tag{19.185}$$

These are dual to the conservation laws for dislocation and disclination densities (19.164) and (19.170).

They can be enforced as Bianchi identities by introducing the stress gauge fields A_{ij} and h_{ij} and writing

$$\begin{aligned} \sigma_{ij} &= \epsilon_{ikl}\partial_k A_{lj} \\ \tau_{ij} &= \epsilon_{ikl}\partial_k h_{lj} - \delta_{ij}A_{ll} - A_{ji}. \end{aligned} \tag{19.186}$$

This allows us to reexpress the energy as

$$E = \int d^3x \left[\frac{1}{4}\left(\sigma_{ij} + \sigma_{ji}\right)^2 + \frac{1}{8l^2}{\tau_{ij}}^2 + A_{ij}\alpha_{ij} + h_{ij}\theta_{ij}\right]. \tag{19.187}$$

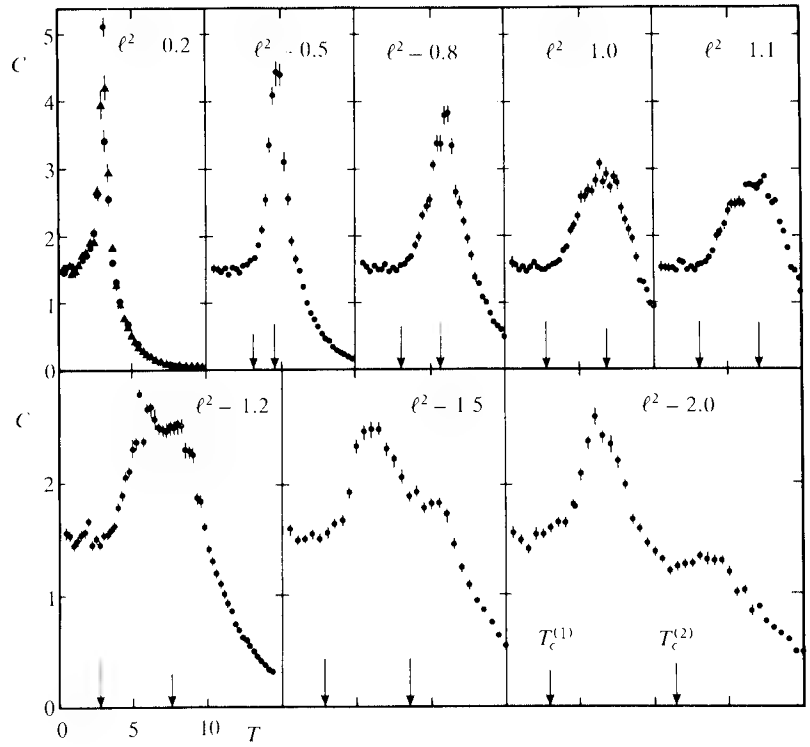

FIGURE 19.6 Separation of first-order melting transition into two successive Kosterlitz-Thouless transitions when increasing the length scale ℓ of rotational stiffness of the defect model.

The stress gauge fields couple locally to the defect densities which are singular on the boundary lines of the Volterra surfaces. In the limit of a vanishing length scale ℓ, τ_{ij} is forced to be identically zero and (19.186) allows us to express A_{ij} in terms of h_{ij}. Then the energy becomes

$$E = \int d^3x \left[\frac{1}{4} \left(\sigma_{ij} + \sigma_{ji} \right)^2 + h_{ij}\eta_{ij} \right] \tag{19.188}$$

where the defect density η_{ij} contains dislocation and disclination lines.

Depending on the length parameter ℓ of rotational stiffness, the defect system was predicted to have either a single first-order transition (for small ℓ), of two successive continuous melting transitions. In the first transitions, dislocation lines proliferate and destroy the translational order, in the second transition, disclination lines proliferate and destroy the rotational order (see Figs. 19.6 and 19.7).

As mentioned in the introduction, the existence of such a scenario was conjectured in two dimensions a long time ago,[12] but the defect models constructed to illustrate this displayed only a single first-order transition.[13] The computer simula-

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[12] D. Nelson and B.I. Halperin, Phys. Rev. B *19*, 2457 (1979); A.P. Young, ibid., 1855 (1979); D. Nelson, Phys. Rev. B *26*, 269 (1982).

[13] W. Janke and H. Kleinert, Phys. Lett. A **105**, 134 (1984); Phys. Lett. A **114**, 255 (1986).

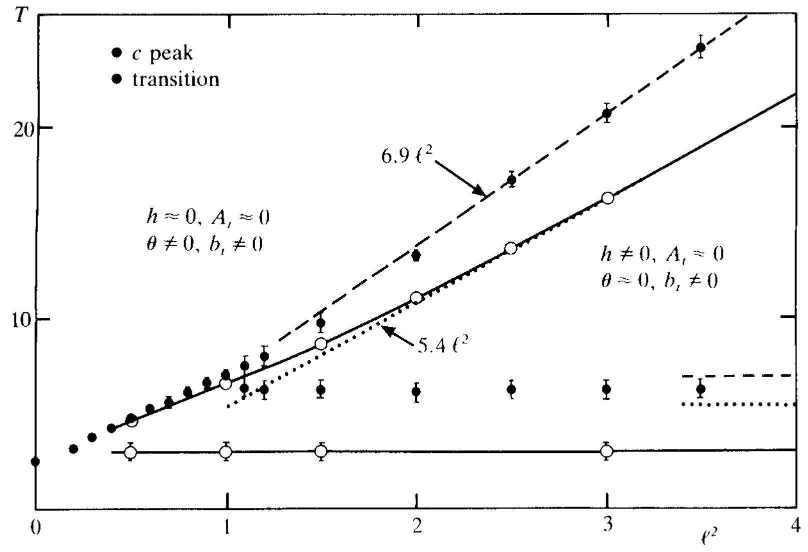

FIGURE 19.7 Phase diagram in the T-ℓ-plane.

tions of the model containing the length parameter ℓ,[14] on the other hand, confirmed the theoretical expectation.[15]

19.4 Charge Confinement

In Section II we have observed the appearance of confining forces caused by the breakdown of vortex gauge invariance: An irrelevant geometric line becomes energetic and creates a linearly rising potential between the endpoints. This mechanism can be used in four spacetime dimensions to construct an abelian theory of quark confinement. In a superconductor, whose ground state contains a condensate of electric charges, magnetic monopoles are confined. To obtain confining force between electric charges, we have to construct a dual theory containing proliferating monopole world lines.

The euclidean field action of such world lines is given by

$$\mathcal{A}=\int d^4x\left\{\frac{1}{4T}\left[F_{\mu\nu}(\mathbf{x})-F^{\rm m}_{\mu\nu}(\mathbf{x})\right]^2+ij_\mu(\mathbf{x})A_\mu(\mathbf{x})\right\} \tag{19.189}$$

where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ is the usual electromagnetic field tensor,

$$j_\mu(\mathbf{x})=e\delta_i(\mathbf{x};L) \tag{19.190}$$

is the current of the electric world lines, and

$$F^{\rm m}_{\mu\nu}=g\frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\delta_{\lambda\kappa}(\mathbf{x};\tilde{S}) \tag{19.191}$$

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[14] W. Janke and H. Kleinert, Phys. Rev. Lett. *61*, 2344 (1988).

[15] H. Kleinert, Phys. Lett. A *130*, 443 (1988).

is the *gauge field of monopoles*. A temperature parameter T has been introduced in analogy with the previous models. At the end, T will be set equal to unity. Instead of discussing the behavior of the theory as a function of the charge e of the electric world lines, we may use the temperature as a parameter. A large temperature corresponds to a large charge e. The δ-function on the surface $\tilde{S}$

$$\delta_{\lambda\kappa}(\mathbf{x};\tilde{S}) = \int d\sigma d\tau \left[\frac{\partial\bar{x}_\mu}{\partial\sigma}\frac{\partial\bar{x}_\nu}{\partial\tau} - (\mu\leftrightarrow\nu)\right]\delta^{(4)}(\mathbf{x}-\bar{\mathbf{x}}(\sigma,\tau)) \tag{19.192}$$

has the property that

$$\partial_\kappa\delta_{\lambda\kappa}(\mathbf{x};\tilde{S}) = \delta_\lambda(\mathbf{x};\tilde{L}) \tag{19.193}$$

where $\tilde{L}$ is the boundary line of $\tilde{S}$. Hence

$$\frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\partial_\nu F^M_{\lambda\kappa} = \tilde{j}_\mu(\mathbf{x}) \tag{19.194}$$

where

$$\tilde{j}_\mu(\mathbf{x}) = g\delta_\mu(\mathbf{x};\tilde{L}) \tag{19.195}$$

is the magnetic current of the monopole world line along $\tilde{L}$. The field energy invariant under monopole gauge transformations $\tilde{S}\to\tilde{S}'$ under which

$$\delta_{\lambda\kappa}(\mathbf{x};\tilde{S}) \to \delta_{\lambda\kappa}(\mathbf{x};\tilde{S}) + \epsilon_{\lambda\kappa\sigma\tau}\partial_\sigma\delta_\tau(\mathbf{x};V) \tag{19.196}$$

where

$$\delta_\tau(\mathbf{x};\tilde{V}) = \epsilon_{\mu\nu\kappa\gamma}\int d\sigma d\tau\lambda\frac{\partial\bar{x}_\nu}{\partial\sigma}\frac{\partial\bar{x}_\mu}{\partial\tau}\frac{\partial\bar{x}_\lambda}{\partial_\lambda}\delta^{(n)}(\mathbf{x}-\bar{\mathbf{x}}(\sigma,\tau,\lambda)) \tag{19.197}$$

is the δ-function on the volume over which $\tilde{S}$ has swept. The vortex gauge field transforms as follows

$$F^{\rm m}_{\mu\nu} \to F^{\rm m}_{\mu\nu} + \partial_\mu\Lambda^{\rm m}_\nu - \partial_\nu\Lambda^{\rm m}_\mu \tag{19.198}$$

where

$$\Lambda^M_\mu = 4\pi q\delta(\mathbf{x};\tilde{V}). \tag{19.199}$$

The gauge functions $\Lambda^{\rm m}_\mu$ can be absorbed into the vector potential

$$A_\mu \to A_\mu + \Lambda^M_\mu. \tag{19.200}$$

The additional interaction term $\int d^4x j_\mu(\mathbf{x})\Lambda^{\rm m}_\mu(\mathbf{x})$ changes by eg times the integral $\int d^4x\delta_\mu(\mathbf{x};L)\delta_\mu(\mathbf{x};\tilde{V})$. The integral is an integer number n counting how many times the line L pierces the volume $\tilde{V}$. Thus, the functional integral of the system

$$Z = \int\mathcal{D}A\sum_{\tilde{S}}e^{-\mathcal{A}} \tag{19.201}$$

picks up a phase factor e^{iegn}. This is an irrelevant factor if

$$eg = 2\pi n, \tag{19.202}$$

which is Dirac's charge quantization condition.[16] By introducing an auxiliary field $\tilde{f}_{\mu\nu}$, the theory can be transformed to the dual form

$$\mathcal{A}=\int d^4x\left[\frac{T}{4}\left(\tilde{F}_{\mu\nu}-\bar{F}^{\rm e}_{\mu\nu}\right)^2+i\int\tilde{j}_\mu\tilde{A}_\mu\right]. \tag{19.203}$$

Here $\tilde{F}_{\mu\nu}=\partial_\mu\tilde{A}_\nu-\partial_\nu\tilde{A}_\mu$ is the field tensor of the magneto electric gauge field $\tilde{A}$ which is locally coupled to the magnetic current $\tilde{j}_\mu(\mathbf{x})$. The world line L of the electric charges are now represented by a gauge field

$$\tilde{F}^{\rm e}_{\mu\nu}=e\frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\delta_{\lambda\kappa}(\mathbf{x};S) \tag{19.204}$$

with some irrelevant surface S whose boundary is L. This field energy is invariant under the dual charge gauge transformations

$$\begin{aligned}\tilde{F}^{\rm e}_{\mu\nu}&\rightarrow\tilde{F}_{\mu\nu}+\partial_\mu\tilde{\Lambda}^{\rm e}_\nu-\partial_\nu\tilde{\Lambda}^{\rm e}_\mu,\\ \tilde{A}_\mu&\rightarrow\tilde{A}_\mu+\tilde{\Lambda}^{\rm e}_\mu.\end{aligned} \tag{19.205}$$

At higher temperatures, the monopole world lines proliferate on account of their entropy. In this phase, they can be described by a disorder field theory and the total action reads

$$\mathcal{A}=\int d^4x\left[\frac{1}{4}\left(\tilde{F}_{\mu\nu}-\tilde{F}^{\rm e}_{\mu\nu}\right)^2+\frac{\tilde{m}_A^2}{2g^2}\left(\partial_\mu\theta-g\tilde{A}_\mu\right)^2\right]. \tag{19.206}$$

By integrating out the angular variables θ of disorder, we are left with a transverse mass term of the $\tilde{A}_\mu$ field

$$\int d^4x\frac{\tilde{m}_A^2}{2}A_\mu^{T2}. \tag{19.207}$$

As a consequence of this, the previously irrelevant surfaces S of the charge gauge fields become massive and give rise to a continuing force between the boundary lines. Going back to the electromagnetic description, the action can be written as

$$\mathcal{A}=\int d^4x\left[\frac{1}{4}\left(F_{\mu\nu}-f_{\mu\nu}\right)^2+ij_\mu A_\mu-i\tilde{A}_\mu\left(\frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\partial_\nu f_{\lambda\kappa}-\tilde{j}_\mu\right)+\frac{1}{2\tilde{m}_A^2}\tilde{j}_\mu^2\right]. \tag{19.208}$$

Here $\tilde{A}_\mu$ plays the role of a Lagrangian multiplier which enforces $f_{\mu\nu}$ to be a gauge field for the monopole world lines $\tilde{L}$.

In the high-temperature phase, the monopoles proliferate and $\tilde{j}_\mu$ can be treated as an ordinary fluctuating transverse field giving rise to the mass term $\frac{\tilde{m}_A^2}{2}\tilde{A}_\mu$. After this, $\tilde{A}_\mu$ can be integrated out and produces a term $1/2\tilde{m}_A^2\left(\frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\partial_\nu f_{s\kappa}\right)^2$. The $f_{\mu\nu}$-field is responsible for the generation of the mass term of the surfaces S in the gauge field description of the electric charges, as can be verified by going again through a duality transformation.

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[16] Dirac uses a field energy with a prefactor $1/4\pi$ in which case e and g have to be replaced by $\sqrt{4\pi e}$ and $\sqrt{4\pi g}$ and the condition reads $2eg=n$.

Near the critical temperature, the fluctuating $\tilde{j}$-currents can be represented by a disorder field theory of the $|\phi|^4$-type and the total action reads (for $T = 1$)

$$\begin{aligned}\mathcal{A} &= \int d^4x\Big[\frac{1}{4}\left(F_{\mu\nu} - f_{\mu\nu}\right)^2 + ij_\mu A_\mu - i\tilde{A}\left(\frac{1}{2}\epsilon_{\mu\nu\lambda\kappa}\partial_\nu f_{\lambda\kappa} - \tilde{j}_\mu\right)\\ &\qquad\qquad + |(\partial_\mu - i\tilde{A}_\mu)\phi|^2 + m^2|\phi|^2 + \frac{g}{2}|\phi|^4\Big].\end{aligned} \tag{19.209}$$

If the monopole charge g is sufficiently small, the disorder field of monopoles [made gauge-invariant as in (19.142)] has a nonzero expectation value and the theory describes electric charges held together by vortex lines. The charges are confined by a linearly rising potential.

Notes and References

The development of this chapter is largely contained in my textbook on this subject
H. Kleinert, *Gauge fields in Condensed Matter*, Vol. I: *Superflow and Vortex Lines, Disorder Fields, Phase Transitions*,
Vol. II: *Stresses and Defects, Differential Geometry, Crystal Defects* , World Scientific, Singapore, 1989.
It was presented as a series of lectures the *Proceedings of a NATO Advanced Study Institute on Formation and Interactions of Topological Defects* t the University of Cambridge, England (cond-mat/9503030) and the textbook

The theory of charge confinement can be found in more detail in
H. Kleinert Int. J. Mod. Phys. A **7**, 4693 (1992) (http://www.physik.fu-berlin.de/~kleinert203); Phys. Lett. B **246**, 127 (1990) (http://www.physik.fu-berlin.de/~kleinert/205); Phys. Lett. B **293**, 168 (1992) (http://www.physik.fu-berlin.de/~kleinert/211).

20

Exactly Solvable O(N)-Symmetric Four-Fermion Theory in $2+\epsilon$ Dimensions

As in the O(N)-symmetric ϕ^4 theory in Section 17.2, there exists also a class of fermionic field theories which can be solved exactly by introducing collective quantum fields of the type discussed in Section 17.1. Consider a large number N of identical fermion fields, coupled by an O(N)-symmetric four-field interaction.

20.1 Scalar Self-Interaction

The Lagrange density reads at finite N:

$$\mathcal{L} = \bar{\psi}_a \left(i\partial\!\!\!/ - m_0 \right) \psi_a + \frac{g_0}{2N} \left(\bar{\psi}_a \psi_a \right)^2 . \tag{20.1}$$

where the index a runs from 1 to N. This model has first been studied in slightly different forms by Anselm, by Vaks and Larkin, and by Nambu and Jona-Lasinio to exhibit the phenomenon of spontanoeus breakdown of chiral symmetry.[1] In a so-called chiral version of th model, the latter authors were the first to point out the existence of a Nambu-Goldstone boson for spontaneously broken continous symmetry. In fact, an extended version of the model can be written down which illustrates the properties of all low-energy phenomena in hadron physics.[2] But recent research has shown that the approximations used in that model are too crude so that the result is not really true.[3] The chiral fluctuations are so strong that the spontanoeusly broken symmetry is restored. This will be discussed in Section 20.10.

The inspiration for studying this model came from the microscopic theory of superconductivity which had just been found by Bardeen, Cooper, and Schrieffer.[4]

A satisfactory definition of the model is only possible in $D = 2+\epsilon$ spacetime dimensions, where it is renormalizable and called the *Gross-Neveu model*.

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[1] See Notes and References.

[2] H. Kleinert, *On the Hadronization of Quark Theories*, Lectures presented at the Erice Summer Institute 1976, in *Understanding the Fundamental Constituents of Matter*, Plenum Press, New York, 1978, A. Zichichi ed., pp. 289-390. http://www.physik.fu-berlin.de/~kleinert/53 .

[3] H. Kleinert and B. Van den Bossche, (hep-ph/9907274).

[4] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. *108*, 1175 (1957).

At the mean-field level, the effective action becomes

$$\Gamma\left[\Psi,\overline{\Psi}\right]=\mathcal{A}\left[\Psi,\overline{\Psi}\right]=\int d^Dx\left[\overline{\Psi}\left(i\partial\!\!\!/-m_0\right)\Psi+\frac{g_0}{2N}\left(\overline{\Psi}_a\Psi_a\right)^2\right] \tag{20.2}$$

and yields an equation of motion

$$\left(i\partial\!\!\!/-m_0+\frac{g_0}{N}\overline{\Psi}_a\Psi_a\right)\Psi_b(x)=0. \tag{20.3}$$

This equation differs in an important physical aspect from the Bose case. It can only have a trivial solution $\Psi_a=0$ for the following reason. In fact, a non-vanishing fermion field expectation in the ground state

$$\Psi_a=\langle 0|\psi_a|0\rangle \tag{20.4}$$

would imply the state $|0\rangle$ to contain a coherent mixture of bosonic and fermionic quantum numbers. Such a state has never been observed in nature. There seems to exist a *superselection rule* forbidding such super-positions. Thus, unlike the Bose field expectation, $\overline{\Psi}_a$ can never become non-zero. Nevertheless, the following discussion will show that the model does exhibit a spontaneous symmetry breakdown, even though the broken symmetry will not be $\hat{O}(N)$ but a discrete one. As before, we shall carry on the discussion in any dimension D.

The generating functional contains linear terms in which the fields are coupled to fermionic anticommuting sources $\eta(x)$ and $\eta(x)$:

$$Z[\eta,\bar{\eta}]=e^{iW[\eta,\bar{\eta}]}=\int\mathcal{D}\psi\mathcal{D}\bar{\psi}e^{i\mathcal{A}[\psi,\bar{\psi}]+i(\bar{\psi}\eta+\text{c.c.})}. \tag{20.5}$$

We introduce a collective field σ fluctuation on the average around $g\bar{\psi}\psi$, as in Eq. (17.4), and rewrite this as

$$Z[\eta,\bar{\eta}]\;=\;\int\mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{D}\sigma e^{i\int d^Dx\left[\bar{\psi}_a(i\partial\!\!\!/-m_0-\sigma)\psi_a+(\bar{\psi}\eta+\text{c.c.})-\frac{N}{2g_0}\sigma^2\right]}. \tag{20.6}$$

The fields ψ can be integrated out according to the rule (10.96), and yield a generating functional containing only the collective field σ:

$$Z[\eta,\bar{\eta}]=\int\mathcal{D}\sigma e^{i\mathcal{A}_{\text{coll}}[\sigma]-\bar{\eta}G_\sigma\eta} \tag{20.7}$$

where

$$\mathcal{A}_{\text{coll}}[\sigma]=N\left\{-\frac{N}{2g_0}\int d^Dx\,\sigma^2-i\text{Tr}\,\log\left[i\partial\!\!\!/-m_0-\sigma\right]\right\}, \tag{20.8}$$

and

$$G_\sigma(x,x')\equiv\frac{i}{i\partial\!\!\!/-m_0-\sigma}(x,x'). \tag{20.9}$$

is the propagator of the fermions in the presence of the collective σ-field, in analogy to (17.6). In the limit $N \to \infty$, the field σ is squeezed into the extremum of the action and we obtain the effective action [compare (17.24)]

$$\begin{aligned} \frac{1}{N}\Gamma[\Sigma,\psi,\bar{\psi}] &= -\frac{1}{2g_0}\int d^Dx\,\Sigma^2(x) - i\mathrm{Tr}\,\log\left[i\partial\!\!\!/ - m_0 - \Sigma(x)\right] \\ &\quad+\frac{1}{N}\int d^Dx\,\Psi_a(x)\left[i\partial\!\!\!/ - m_0 - \Sigma(x)\right]\Psi_a(x) \end{aligned} \tag{20.10}$$

The extremum of $\Gamma[\Sigma,\psi,\bar{\psi}]$ yields the equtions of motion,

$$\left[i\partial\!\!\!/ - m_0 - \Sigma(x)\right]\Psi_a(x) = 0, \tag{20.11}$$

and

$$\Sigma(x) = g_0\mathrm{tr}\left(\frac{i}{i\partial\!\!\!/ - m_0 - \Sigma}\right)(x,x) - \frac{1}{N}g_0\bar{\Psi}_a\Psi_a(x), \tag{20.12}$$

where tr indicates a trace over the Dirac indices. As argued above, the field expectation $\Psi_a(x)$ must vanish, so that the only equation to be solved is

$$\Sigma(x) = g_0\mathrm{tr}\left(\frac{i}{i\partial\!\!\!/ - m_0 - \Sigma}\right)(x,x). \tag{20.13}$$

It is called *gap equation* because of its first analogous appearance in the theory of superconductivity.

Thus, as far as the extremum is concerned, we may study only the purely collective part of the exact action

$$\frac{1}{N}\Gamma[\Sigma] = -\frac{1}{2g_0}\int d^Dx\,\Sigma^2 - i\mathrm{Tr}\,\log\left(i\partial\!\!\!/ - m_0 - \Sigma\right). \tag{20.14}$$

Let us seek for an extremal constant solution Σ_0 Then the gap equation reduces to

$$\begin{aligned} \Sigma_0 &= ig_0\,\mathrm{tr}\int\frac{d^Dp}{(2\pi)^D}\frac{p\!\!\!/ + m_0 + \Sigma_0}{p^2 - (m_0+\Sigma_0)^2} \\ &= \mathrm{tr}\,(1)\;g_0\int\frac{d^Dp_E}{(2\pi)^D}\frac{m_0+\Sigma_0}{p_E^2 + (m_0+\Sigma_0)^2}. \end{aligned} \tag{20.15}$$

The Dirac matrices have disappeared, except for the unit matrix inside the trace. This makes it possible to use this equation in any desired number dimensions. We only need to know the dimension of the Dirac matrices, which is $2^{D/2}$ for even D. In this form, Eq. (20.4) may be extrapolated analytically to any non-integer value of D.

For a constant Σ, the effective action gives rise to an effective potential

$$\frac{1}{N}v(\Sigma) = -\frac{1}{NV}\Gamma[\Sigma] = \frac{1}{2g_0}\Sigma^2 - \mathrm{tr}\,(1)\frac{1}{2}\int\frac{d^Dp_E}{(2\pi)^D}\log\left[p_E^2 + (m_0+\Sigma)^2\right], \tag{20.16}$$

where $V \equiv \int d^D x$ is the total volume of the system. The last term is obtained from the Tr log in (20.10) by the following calculation

$$\begin{aligned}
\int \frac{d^D p}{(2\pi)^D} \log(\not p - m_0 - \Sigma) &= \frac{1}{2}\int \frac{d^D p}{(2\pi)^D}\left[\log(\not p - m_0 - \Sigma) + \log(-\not p - m_0 - \Sigma)\right] \\
&= \frac{1}{2}\int \frac{d^D p}{(2\pi)^D} \log\left[-p^2 + (m_0+\Sigma)^2\right] \\
&= \frac{i}{2}\int \frac{d^D p_E}{(2\pi)^D} \log\left[p_E^2 + (m_0+\Sigma)^2\right].
\end{aligned}$$

The integral is performed with the help of formula (9.133), and yields

$$\frac{1}{N}v(\Sigma) = \frac{1}{2g_0}\Sigma^2 - 2^{D/2-1}\mu^{D-2}\frac{1}{2}S_D\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}\left(\frac{m_0+\Sigma}{\mu}\right)^D \mu^2. \tag{20.17}$$

We have introduced, as usual, and arbitrary mass scale μ, which will enable us to study the theory in the limit $m_0 = 0$.

We now focus attention upon the dimensional neighbourhood of $D = 2$ spacetime dimensions, setting

$$D = 2+\epsilon, \quad \text{with} \quad \epsilon > 0. \tag{20.18}$$

Then

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}\left[\frac{\Sigma^2}{g_0\mu^\epsilon} - b_\epsilon\left(\frac{m_0+\Sigma}{\mu}\right)^{2+\epsilon}\mu^2\right], \tag{20.19}$$

where the constant b_ϵ stands for

$$\begin{aligned}
b_\epsilon &= \frac{2}{D}2^{\epsilon/2}S_D\Gamma(D/2)\Gamma(1-D/2) = \frac{2}{D}\frac{1}{(2\pi)^{D/2}}\Gamma(1-D/2) \\
&= \frac{2}{2+\epsilon}\frac{1}{(2\pi)^{1+\epsilon/2}}\Gamma(-\epsilon/2).
\end{aligned} \tag{20.20}$$

For small ϵ, the constant b_ϵ behaves like

$$b_\epsilon \sim -\frac{1}{\epsilon\pi}\left[1 - \frac{\epsilon}{2}\log\left(2\pi e^{-\gamma}\right)\right] + \mathcal{O}(\epsilon). \tag{20.21}$$

Therefore, the bare parameters must somehow diverge if the theory is to remain finite in the limit $\epsilon \longrightarrow 0$.

For simplicity, consider at first the massless case, $m = 0$. Then a renormalized coupling constant can be defined via

$$\frac{1}{g_0\mu^\epsilon} - b_\epsilon = \frac{1}{g}. \tag{20.22}$$

The limit $\epsilon \to 0$ can now be taken at a finite g and we obtain the renormalized potential

$$\frac{1}{N}v(\Sigma) \to \frac{1}{2}\left[\frac{\Sigma^2}{g} + \frac{\Sigma^2}{\pi}\log\left(\frac{\Sigma}{\mu}\right)\right]. \tag{20.23}$$

For arbitrary $0 < \epsilon < 4$, we may write a renormalized v as

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}\left\{\frac{\Sigma^2}{g} + b_\epsilon\Sigma^2\left[1 - \left(\frac{\Sigma}{\mu}\right)^\epsilon\right]\right\} \tag{20.24}$$

which reduces to (20.23) for $\Sigma \to \Sigma_0$.

Let us now study the possibility of a nontrivial solution $\Sigma = \Sigma_0$ for the gap equation (20.15) at $m_0 = 0$. There is no need to perform the integral in that equation since the result can immediately be btained from the minimum of $v(\Sigma)$. Thus we simply differentiate (20.19) for $m_0 = 0$, and obtain

$$1 = g_0\mu^\epsilon b_\epsilon\frac{2+\epsilon}{2}\left(\frac{\Sigma_0}{\mu}\right)^\epsilon. \tag{20.25}$$

In the renormalized version (20.24) this reads

$$1 = gb_\epsilon\left[\left(1+\frac{\epsilon}{2}\right)\left(\frac{\Sigma_0}{\mu}\right)^\epsilon - 1\right], \tag{20.26}$$

and becomes in the limit $\epsilon \to 0$:

$$1 = -\frac{1}{\pi}g\left(\frac{1}{2} + \log\frac{\Sigma_0}{\mu}\right). \tag{20.27}$$

The vacuum expectation of the collective field is therefore given by

$$\Sigma_0 = \mu e^{-(1/2+\pi/g)}. \tag{20.28}$$

The question arises whether this non-trivial solution corresponds to the true ground state of the problem. For this, we differentiate $v(\Sigma)$ once more, and find

$$\frac{1}{N}v''(\Sigma) = \frac{1}{g_0} - b_\epsilon\left(D-1\right)\frac{D}{2}\Sigma^\epsilon. \tag{20.29}$$

Inserting (20.26), this becomes

$$\frac{1}{N}v''(\Sigma) = -\frac{1}{g_0}(D-2) = -\epsilon b_\epsilon\left(1+\epsilon/2\right)\Sigma_0^\epsilon, \tag{20.30}$$

which is positive for $D > 2$ if

$$g_0 < 0. \tag{20.31}$$

What does this condition mean for the renormalized coupling g? Using (20.22), we see that $g_0 < 0$ and $g_0 > 0$ amount to $g > g^*$ and $g < g^*$, respectively, with

$$g^* \equiv -b_\epsilon^{-1} = \epsilon\pi. \tag{20.32}$$

This is a critical coupling constant above which the model has a phase with a nonvanishing field expectation Σ_0. If the renormalized coupling lies below g^*, the bare coupling constant is positive and only the trivial solution $\Sigma_0 = 0$ has a positive $v''(\Sigma_0)$ indicating stability.

What are the physical properties of the two solutions? Looking back at the effective action (20.107), we see that Σ_0 increased the fermion mass term to $M = m_0 + \Sigma_0$. In the present zero-m_0 case,

$$M = \Sigma_0. \tag{20.33}$$

We therefore conclude that for $g < g^*$, the massless input fermions remain massless. For $g > g^*$, on the other hand, the massless fermions aquire a mass $M = \Sigma_0$ from the fluctuations. We observe a *spontaneous generation of a fermion mass*. The result may also be phrased differently: In the weak-coupling phase with $g < g^*$-phase, the fermions keep their initial long-range correlations, in the strong-couling phase with $g > g^*$, however, the spontaneously generated mass limits their correlation functions to a range $1/M$.

20.2 Spontanous Symmetry Breakdown

The spontaneous mass generation is closely related to the fact that the model displays, for zero initial mass, the phenomenon of spontaneous symmetry breakdown (recall Chapters 15, 17). Indeed, for $m_0 = 0$, the Lagrangian (20.1) possesses an additional symmetry called γ_5-*invariance*. In two dimensions we may choose the following γ-matrices:

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma^1, \qquad \gamma^1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\sigma^2 \tag{20.34}$$

which satisfy

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} = 2\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^{\mu\nu} \tag{20.35}$$

The hermitian γ^5-matrix is defined in analogy with the four dimensional case in Eq. (3.495) as

$$\gamma^5 = \frac{1}{2!}\epsilon_{\mu\nu}\gamma^\mu\gamma^\nu = \gamma^0\gamma^1, \tag{20.36}$$

where $\epsilon_{\mu\nu}$ is the completely antisymmetric tensor with $\epsilon_{01} = 1$. In the representation (20.34), γ_5 is equal to the Pauli matrix σ_3:

$$\gamma^5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{20.37}$$

We now introduce γ_5-transformations T_{γ_5} as follows:

$$\psi \xrightarrow[T_{\gamma_5}]{} \gamma_5\psi \tag{20.38}$$

which satisfies $T_{\gamma_5}^2 = 1$. Under T_{γ_5}:

$$\bar\psi \xrightarrow[T_{\gamma_5}]{} \psi^\dagger\gamma_5\gamma_0 \to -\bar\psi\gamma_5. \tag{20.39}$$

Hence:

$$\begin{aligned} \bar\psi\psi &\to -\bar\psi\psi \\ \bar\psi\gamma^\mu\psi &\to \bar\psi\gamma^\mu\psi \end{aligned} \tag{20.40}$$

If the bare mass m_0 in (20.1) is zero, the Lagrangian is invariant under T_{γ_5}.

Also the action in the exponents of (20.6) and (20.7) are invariant, if we assign to $\sigma \sim g\bar\psi\psi$, in accordance with (20.36), (20.38) the transformation

$$\sigma \xrightarrow[T_{\gamma_5}]{} -\sigma. \tag{20.41}$$

Thus the $m_0 = 0$ collective action (20.8) is symmetric in σ. It is precisely this γ_5 symmetry which is broken by the non-vanishing expectation value $\langle\sigma\rangle = \Sigma^0$. We may compare this result with our Bose discussion in Section 17.4 of the last Chapter. There we found that the continuous O(N) symmetry could not be broken in less or equal two dimensions due to fluctuations, due to the fact that such a phase would contain massless Nambu-Goldstone bosons in two dimensions, whose correlation functions diverge at any distance. Here we see, in contrast, that a discrete symmetry can be broken in two dimensions.

20.3 Dimensionally Transmuted Coupling Constant

It is worth pointing out an important structural property of the final result: The characteristic parameter of the two-dimensional system is the fermion mass which is determined from the coupling strength and the arbitrary mass parameter μ via (20.28), (20.33) as

$$M = \mu e^{-(1/2+\pi/g)}. \tag{20.42}$$

The original theory with $m_0 = 0$ had only a single free parameter, namely the coupling strength g_0. The auxiliary mass parameter μ was only introduced for the purpose of renormalizing the theory in the massless case. The renormalized coupling g depends on the choice of μ, and (20.22) should more explicitly be written as

$$\frac{1}{g_0\mu^\epsilon} - b_\epsilon = \frac{1}{g(\mu)}. \tag{20.43}$$

In this way, a system with a single parameter g_0 has been recharacterized by two parameters μ and $g(\mu)$.

This increase of parameters is certainly an artefact. There must be a relation between μ and $g(\mu)$ such that different pairs $(\mu, g(\mu))$ correspond to the same set of Green's functions, i. e., to the same physical theory. Indeed, such a relation follows from (20.22). At a fixed g_0, we can plot curves in the (μ, g) plane which correspond to one and the same theory. In the limit $\epsilon \longrightarrow 0$ this relation between μ and g has a subtlety. It goes over into the mass relation (20.42).

The fermion mass is a physically observable finite quantity. There are infinitely many pairs of parameter μ and coupling $g(\mu)$ which lead to the same fermion mass, and this mass is the most economic single parameter by which all properties of the theory can be expressed. Let us illustrate this by reexpressing the potential (20.23) in terms of M. For this we write the renormalized gap equation in the form (with $\Sigma_0 = M$)

$$\frac{\pi}{g} + \frac{1}{2} + \log\frac{M}{\mu} = 0. \tag{20.44}$$

Multiplying this by $\Sigma^2/2$, and subtracting the result from the potential (20.23), we find

$$\frac{1}{N}v(\Sigma) = \frac{\Sigma^2}{2\pi}\left(\log\frac{\Sigma}{M} - \frac{1}{2}\right). \tag{20.45}$$

This has indeed the desired property that neither μ nor $g(\mu)$ appear but only the single parameter M. The same property can, of course, be verified in $D > 2$ dimensions. Here we may combine (20.26) with (20.24) and find

$$\begin{aligned}\frac{1}{N}v(\Sigma) &= \frac{\mu^\epsilon}{2}\left[\frac{\Sigma^2}{g_0\mu^\epsilon} - b_\epsilon\left(\frac{\Sigma}{\mu}\right)^{2+\epsilon}\mu^2\right] \\ &= \frac{M^\epsilon}{2}b_\epsilon\Sigma^2\left[1 + \frac{\epsilon}{2} - \left(\frac{\Sigma}{M}\right)^\epsilon\right].\end{aligned} \tag{20.46}$$

For $\epsilon \longrightarrow 0$, this reduces to (20.45).

20.4 Scattering Amplitude for Fermions

We calculate the scattering amplitude for fermions. As we know from the discussion in the Bose case, this is given entirely by the exchange of Σ-propagators. These can be extracted from the effective action (20.10) with $m_0 = 0$ by forming the second functional derivative at Σ_0 [compare the discussion leading to (17.135) and (17.136)]. The quadratic piece in $\Sigma' \equiv \Sigma - \Sigma_0 = \Sigma - M$ is

$$\delta^2\Gamma = -\frac{N}{2}\left[\frac{1}{g_0}\int d^Dx\,\Sigma'^2 + i\,\mathrm{Tr}\left(\frac{i}{i\partial\!\!\!/ - M}\Sigma'\frac{i}{i\partial\!\!\!/ - M}\Sigma'\right)\right]. \tag{20.47}$$

From this we extract the propagator of the σ'-fluctuations in momentum space

$$G_{\sigma'\sigma'}(q) = -\frac{1}{N}\frac{i}{g_0^{-1} + \Pi(q)}, \tag{20.48}$$

where the self-energy of the σ' field is given by the integral

$$\begin{aligned} \Pi(q) &= i \operatorname{tr} \int \frac{d^D k}{(2\pi)^D} \frac{i}{\not{k} - M + i\eta} \frac{i}{(\not{k} - \not{q}) - M + i\eta} \\ &= -i \operatorname{tr} \int \frac{d^D k}{(2\pi)^D} \frac{[(\not{k} + M)(\not{k} - \not{q} + M)]}{(k^2 - M^2)\left[(k-q)^2 - M^2\right]}. \end{aligned} \tag{20.49}$$

with the momenta illustrated in the Feynman diagram shown in Fig. 20.1

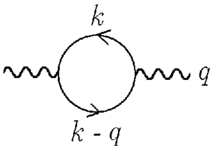

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FIGURE 20.1 One-loop Feynman diagram in the inverse propagator of the σ'-field.

Forming the trace and going to euclidean momentum space yields

$$\Pi(q) = -2^{D/2} \int \frac{d^D k_E}{(2\pi)^D} \frac{k(k-q)_E - M^2}{\left(k_E^2 + M^2\right)\left[(k-q)_E^2 + M^2\right]}, \tag{20.50}$$

In the last line we have gone to the euclidean form. The denominator can be treated with the help of the Feynman formula (9.154), and we may write [compare (9.157)]

$$\Pi(q) = -2^{D/2} \int \frac{d^D k_E}{(2\pi)^D} \int_0^1 dx \frac{k(k-q)_E - M^2}{\left(k_E^2 - 2k_E q_E x + q_E^2 x + M^2\right)^2}. \tag{20.51}$$

The integrand can be rearranged to

$$\frac{(k-qx)_E^2 + (k-qx)_E q_E (2x-1) - q_E^2 x(1-x) - M^2}{\left[(k-qx)_E^2 + q_E^2 x(1-x) + M^2\right]^2}. \tag{20.52}$$

Upon integration over the shifted momentum $k' \equiv k - qx$, the second term in the numerator will vanish since it is odd in k'. We therefore remain with the integral

$$\begin{aligned} \Pi(q) = -2^{D/2} \int_0^1 dx \int \frac{d^D k_E}{(2\pi)^D} \\ \times \left\{ \frac{1}{k_E^2 + q_E^2 x(1-x) + M^2} - 2\frac{M^2 + q_E^2 x(1-x)}{\left[k_E^2 + q_E^2 x(1-x) + M^2\right]^2} \right\}. \end{aligned} \tag{20.53}$$

This can be integrated using formulas (9.122), leading to

$$\begin{aligned}\Pi(q) &= -2^{D/2}\bar{S}_D\left[\frac{1}{2}\frac{\Gamma(D/2)\Gamma(1-D/2)}{\Gamma(1)}-2\,\frac{1}{2}\frac{\Gamma(D/2)\Gamma(2-D/2)}{\Gamma(2)}\right]\\ &\times\int_0^1 dx\left[q_E^2x(1-x)+M^2\right]^{D/2-1} \qquad (20.54)\\ &= -2^{D/2-1}\bar{S}_D(D-1)\Gamma(D/2)\Gamma\left(1-D/2\right)M^\epsilon\int_0^1 dx\left[\frac{q_E^2}{M^2}x(1-x)+1\right]^{D/2-1}\\ &= -\frac{D(D-1)}{2}b_\epsilon M^\epsilon\int_0^1 dx\left[\frac{q_E^2}{M^2}x(1-x)+1\right]^{-\epsilon/2}, \qquad (20.55)\end{aligned}$$

where we have introduced the parameter b_ϵ of (20.20). Inserting this into (20.47) we obtain the propagator in terms of the renormalized coupling g:

$$\begin{aligned}G_{\sigma'\sigma'} &= -\frac{i}{N}\mu^{-\epsilon}\left\{\frac{1}{g_0\mu^\epsilon}-\frac{D(D-1)}{2}b_\epsilon\left(\frac{M}{\mu}\right)^\epsilon\int_0^1 dx\left[\frac{g_\epsilon^2}{M^2}x(1-x)+1\right]^{\epsilon/2}\right\}^{-1}\\ &= -\frac{i}{N}\mu^{-\epsilon}\left(\frac{1}{g}+b_\epsilon\left\{1-\frac{D(D-1)}{2}\left(\frac{M}{\mu}\right)^\epsilon\int_0^1 dx\left[\frac{q_E^2}{M^2}x(1-x)+1\right]^{\epsilon/2}\right\}\right)^{-1}. \qquad (20.56)\end{aligned}$$

The expression in the last curly brackets behaves for small ϵ like

$$\begin{aligned}&1-\left(1+\frac{\epsilon}{2}\right)(1+\epsilon)\left\{1+\frac{\epsilon}{2}\int_0^1 dx\log\left[\frac{q_E^2}{M^2}x(1-x)+1\right]+\epsilon\log\frac{M}{\mu}\right\}\\ &\qquad= -\frac{\epsilon}{2}\left\{\left[\int_0^1 dx\log\left(\frac{q_E^2}{M^2}x(1-x)+1\right)\right]+3+2\log\frac{M}{\mu}\right\}, \qquad (20.57)\end{aligned}$$

so that the big parenthesis of (20.48) become, in $D=2$ dimensions,

$$\left(\frac{1}{g}+\frac{1}{2\pi}\left\{\int_0^1 dx\log\left[\frac{q_E^2}{M^2}x(1-x)+1\right]+3+2\log\frac{M}{\mu}\right\}\right). \qquad (20.58)$$

This result can be expressed completely in terms of M. For this purpose, we subtract again the gap equation (20.27) and find

$$\frac{1}{2\pi}\int_0^1 dx\left\{\log\left[\frac{q_E^2}{M^2}x(1-x)+1\right]+2\right\} \qquad (20.59)$$

and the σ'-propagator takes the desired form

$$\begin{aligned}G_{\sigma'\sigma'}(q) &= -\frac{i}{N}\frac{1}{g_0^{-1}+\Pi(q)}\\ &= -\frac{i}{N}\frac{2\pi}{\displaystyle\int_0^1 dx\log\left[\frac{q_E^2}{M^2}x(1-x)+1\right]+2}. \qquad (20.60)\end{aligned}$$

The integral in the denominator has been solved before in Eqs. (9.169)–(9.172)], where we found, with $z \equiv q_E^2/M^2$,

$$J(z) = \int_0^1 dx \log\left[zx(1-x)+1\right] = -2 + 2\theta\coth\theta, \tag{20.61}$$

where

$$\theta = \operatorname{atanh}\sqrt{\frac{z}{z+4}} = \operatorname{atanh}\sqrt{\frac{q_E^2}{q_E^2+4M^2}}, \quad \sinh\theta = \sqrt{\frac{z}{4}} = \sqrt{\frac{q_E^2}{4M^2}}. \tag{20.62}$$

The function $J(z)$ is monotonously increasing in q_E^2, with the minimum lying at the origin, as shown in Fig. 20.2. The propagator itself starts out, in momentum space,

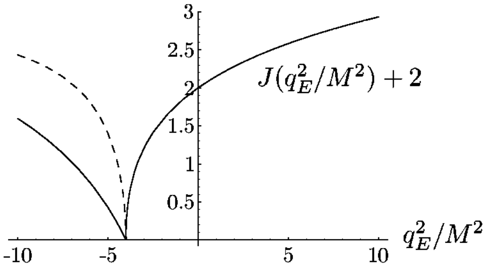

FIGURE 20.2 The function $J(z)+2$ in the denominator pf the σ'-propagator (20.60). FOr $z < -4$, the curve shows the real, the dashed curve the imaginary part.

with

$$G_{\sigma'\sigma'}(q)\big|_{q_E^2=0} = -i\frac{\pi}{N}, \tag{20.63}$$

and has a monotonously decreasing size for growing euclidean momentum q_E.

We may now ask whether there exists a scalar ground state in the fermion antifermion scattering amplitude, which is usually called σ-particle in the analogy with a resonance of $\pi^\dagger\pi^-$ in the proton proton scattering amplitude which is seen at roughly 700 MeV (and which is the origin of using the name σ for the collective field $\sigma \sim \bar{\psi}\psi$. This particle would have to manifest itself in a pole in the propagator $G_{\sigma'\sigma'}(q_E^2)$ at timelike q^2, i. e., at a negative value of $q_E^2 = -s = -M_\sigma^2$. Indeed, the denominator (20.61) is seen to vanish for

$$s = 4M^2 \tag{20.64}$$

as can be seen by continuing (20.61) to $0 < s < 4M^2$ using

$$\theta\coth\theta = \bar\theta\coth\bar\theta \tag{20.65}$$

In terms of s, the parameter θ is given by

$$\theta = \arctan\sqrt{\frac{s}{s-4M^2}}, \quad \sin\theta = \sqrt{\frac{s}{4M^2}}. \tag{20.66}$$

Close to $4M^2$ the propagator behaves like

$$G_{\sigma'\sigma'} = -\frac{2i}{N}\sqrt{\frac{s}{s-4M^2}}. \tag{20.67}$$

Thus we see that there is no proper particle pole at $s = 4M^2$, but only a branch cut which runs from $s = 4M^2$ to infinity. Such a cut is present in every scattering amplitude and commonly referred to as the *elastic cut*. This is an artifact of the leading large-N approximation investigated in the present discussion. For finite N, the Green function does have a proper bound-state pole before the cut starts.

As in the effective potential, there is only the fermion mass M which characterizes the theory, instead of the bare coupling g_0, since the latter becomes undefined for $\epsilon \to 0$. The fermion mass M is independent on the particular renormalization procedure. It may come as a surprise that a dimensionless quantity g_0 has been replaced by quantity with the dimension of a mass. This process is often referred to as *dimensional transmutation*. It was first observed in the microscopic theory of superconductivity. There are many superconductors with different coupling strenghts g and mass parameters μ (which are a characteristic for the phonon spectrum; see Chapter 16), but there is only one quantity specific for the superconductivity properties which is the critical temperature T_c. Theories with the same T_c are identical superconductors independent on what g or μ they were derived from. There is one important difference, however, between the different cases: In the fundamental Lagrangian (20.1), the mass parameter μ and the associated $g(\mu)$ are not detectable separately by any physical experiment. Only their combination M is. In a superconductor, on the other hand, both quantities are properties of the microscopic substructure and can both be measured. This points at an important physical aspect of the renormalization procedure: Every theory which requires renormalization of the coupling constant has a redundancy in its parameterization with a mass parameter μ and a renormalized coupling constant $g(\mu)$. This redundancy cannot be resolved at the level of the theory itself. But there may be a more microscopic theory in which both parameters μ and $g(\mu)$ acquire a separate physical significance. Until now, theoretical physics has gone precisely this way. Every theory which was initially considered to be microscopic turned later out to be a phenomenological description of even more microscopic substructures.

The reader may wonder how this description applies to the phase at small coupling constants $g < g^*$ or $g^0 > 0$, where the fermions remain massless and there are long-range correlations. The potential may still be parametrized in the form (20.19), (20.24) with $m_0 = 0$:

$$\begin{aligned}\frac{1}{N}v(\Sigma) &= \frac{\mu^\epsilon}{2}\left[\frac{\Sigma^2}{g_0\mu^\epsilon} - b_\epsilon\left(\frac{\Sigma}{\mu}\right)^{2+\epsilon}\mu^2\right]\\ &= \frac{\mu^2}{2}\left\{\frac{\Sigma^2}{g} - b_\epsilon\Sigma^2\left[\left(\frac{\Sigma}{\mu}\right)^\epsilon\mu^2 - 1\right]\right\}.\end{aligned} \tag{20.68}$$

There remains the arbitrary mass parameter μ with the renormalized coupling g depending on the choice of μ. There is now no fermion mass in terms of which the result can be expressed in a renormalization independent fashion. Nevertheless, it is still possible to substitute the pair of parameters $\mu, g(\mu)$, by a single one whose dimension is mass. For this we may simply turn the sign of Eq. (20.25) and define M by

$$1 \equiv -g_0 \mu^\epsilon b_\epsilon \frac{D}{2} \left(\frac{M}{\mu} \right)^\epsilon . \tag{20.69}$$

Now $v(\Sigma) =$ can be rewritten as

$$\frac{1}{N} v(\Sigma) = -\frac{M^\epsilon}{2} b_\epsilon \Sigma^2 \left[\frac{D}{2} + \left(\frac{\Sigma}{M} \right)^\epsilon \right], \tag{20.70}$$

and M is a measure for the deviation of the potential from its quadratic shape. The minimum lies at the origin corresponding to the massless fermions.

Note that this potential exists only for ϵ truly larger than zero. For $\epsilon \to 0$, there is no finite limit. This is due to the fact that only for negative g_0, $1/g_0\mu^\epsilon - b_\epsilon$ can be compensated to become a finite quantity $1/g$ in the limit $\epsilon \to 0$.

If we calculate (20.58) for vanishing fermion mass, we obtain

$$\begin{aligned} G_{\sigma'\sigma'}(q) &= -\frac{i}{N} \mu^{-\epsilon} \left\{ \frac{1}{g_0 \mu^\epsilon} - \frac{D(D-1)}{2} b_\epsilon \left(\frac{q_E^2}{\mu^2} \right)^{\epsilon/2} \int_0^1 dx \, [x(1-x)]^{\epsilon/2} \right\}^{-1} \\ &= -\frac{i}{N} \mu^{-\epsilon} \left\{ \frac{1}{g_0 \mu^\epsilon} - \frac{D(D-1)}{2} b_\epsilon \frac{\Gamma^2(1+\epsilon/2)}{\Gamma(2+\epsilon)} \left(\frac{q_E^2}{\mu^2} \right)^{\epsilon/2} \right\}^{-1} . \end{aligned} \tag{20.71}$$

This may be expressed in terms of the auxiliary mass parameter (20.69) as

$$G_{\sigma'\sigma'}(q) = \frac{i}{N} \left(\frac{D}{2} b_\epsilon M^\epsilon \right)^{-1} \left[1 + \frac{\Gamma^2(1+\epsilon/2)}{\Gamma(1+\epsilon)} \left(\frac{q_E^2}{M^2} \right)^{\epsilon/2} \right]^{-1} . \tag{20.72}$$

It should be pointed out that if we had calculated propagator $G_{\sigma'\sigma'}(q)$ by expanding the action around the wrong ground state solution, say $\Sigma_0 = 0$ for $g_0 < 0$, $g > g^*$, the resulting propagator would show this mistake. This is seen directly in Eq. (20.71), which is singular at euclidean momentum by having an unphysical tachyon

$$q_E^2 = \left[\frac{1}{g_0 b_\epsilon} \frac{\Gamma(2+\epsilon)}{\Gamma^2(1+\epsilon/2)} \frac{2}{D(D-1)} \right]^{2/\epsilon} . \tag{20.73}$$

This may also be expressed in terms of renormalized quantities as

$$\frac{q_E^2}{\mu^2} = \left[\left(1 + \frac{1}{g b_\epsilon} \right) \frac{\Gamma(2+\epsilon)}{\Gamma(1+\epsilon/2)} \frac{2}{D(D-1)} \right]^{2/\epsilon} . \tag{20.74}$$

When going to Minkowski space this amounts to a particle pole at

$$q^2 = -q_E^2.$$

This is similar to the situation in ϕ^4 theory in four dimensions. Also there we found such a particle with an imaginary mass which travels faster than the speed of light and is therefore unphysical (tachyon). There it appeared for very large q^2, here for very small q^2. Since a tachyon can have states with arbitrary negative energy, there must be another ground state for the theory which lies lower than the zero-field configuration.

It can be argued that for finite N, positive couplings g_0 correspond to another interesting physical phase for which the collective field $\sigma \sim (g_0/N)\bar{\psi}_a\psi_a$ is no longer appropriate. Instead, a field proportional to $\psi_a\psi_a$ allows now for an economic description. This will becomes clearer after the next section.

There is one more observation we should make in the massive phase. We may express the potential (20.24) also in terms of g^*, and find the form

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}\frac{1}{g}\left[\left(1-\frac{g}{g^*}\right)\Sigma^2 + \frac{g}{g^*}\left(\frac{\Sigma}{\mu}\right)^\epsilon\right]\epsilon^2. \tag{20.75}$$

This form exhibits very nicely the unstable origin for $g > g^*$ and the stabilization due to the term $\Sigma^{2+\epsilon}$. The potential looks very similar to the previously discussed ϕ^4 theory. In fact, for $\epsilon \longrightarrow 2$ ($D \longrightarrow 4$) it takes exactly this form. The minimum lies at $\Sigma = \Sigma_0 = M$, where M is the fermion mass

$$\frac{M}{\mu} = \left[\frac{2}{D}\frac{g^*}{g}\left(\frac{g}{g^*}-1\right)\right]^{1/\epsilon} \tag{20.76}$$

in terms of which the potential may be written in a natural parametrization

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}M^2\frac{1}{g}\left(\frac{g}{g^*}-1\right)\left[-\left(\frac{\Sigma}{M}\right)^2 + \frac{2}{D}\left(\frac{\Sigma}{M}\right)^D\right]. \tag{20.77}$$

The mass scale ν can be replaced by the physical mass at infinite g

$$M_\infty = \left(\frac{2}{D}\right)^{1/\epsilon}. \tag{20.78}$$

Then (20.76) reads

$$\frac{M}{M_\infty} = \left(1-\frac{g^*}{g}-1\right)^{1/\epsilon}. \tag{20.79}$$

We argued before that g, g^* play the role of temperature T and critical temperature T_c in surface layers. There the mass goes with

$$\frac{M}{\mu} \propto \left(\frac{T}{T_c}-1\right)^{1/\epsilon} \hat{=} \left(\frac{g}{g^*}-1\right)^{1/\epsilon}. \tag{20.80}$$

It vanishes at the critical point in which case v takes on a pure power behavior

$$\frac{1}{N}v(\Sigma) \underset{\Sigma\to 0}{\sim} \mu^D \left(\frac{\Sigma}{\mu}\right)^D . \tag{20.81}$$

This power can also be seen at arbitrary T if Σ is increased to be much larger than the mass scale M [ultraviolet (UV) limit of the theory].

Note that in the opposite limit of small Σ [infrared (IR) limit], the power behavior is

$$\frac{1}{N}v(\Sigma) \underset{\Sigma\to 0}{\sim} \Sigma^2 \tag{20.82}$$

which corresponds to the $g \to 0$, i.e., the free-field limit of the theory. One says, the theory behaves IR free. Such UV and IR power behaviors are typical at a critical point. They have been the subject of extended experimental and theoretical investigation over the past decade. It will be worthwile to dedicate the next chapter to the corresponding physical phenomena.

20.5 Nonzero Bare Fermion Mass

Before we come to that, let us shortly indicate what happens to this model if there is a fermion mass from the beginning, a case which we discarded for the sake of simplicity. We may assume m_0 to be positive, since otherwise its sign can be changed by a simple γ_5 transformation under which $m_0\bar{\psi}\psi \to -m_0\bar{\psi}\psi$. Differentiating (20.19), we obtain the gap equation

$$\frac{\Sigma_0}{g_0\mu^\epsilon} = \left(1+\frac{\epsilon}{2}\right) b_\epsilon \left(\frac{m_0+\Sigma_0}{\mu}\right)^{1+\epsilon} \mu \tag{20.83}$$

which has a solution $\Sigma_0 > 0$ for $g_0 < 0$ and $-m_0 < \Sigma_0 < 0$ for $g_0 > 0$. In other words, for repulsive interaction the mass becomes larger and for attractive interaction smaller. The second derivative is

$$\frac{1}{N}v''(\Sigma) \;=\; \mu^\epsilon \left[\frac{1}{g_0\mu^\epsilon} - b_\epsilon \frac{D}{2}(D-1)\left(\frac{m_0+\Sigma}{\mu}\right)^{D-2}\right], \tag{20.84}$$

and at the solution Σ_0 of the gap equation (20.83):

$$\begin{aligned} \frac{1}{N}v''(\Sigma_0) &= \mu^\epsilon \frac{1}{g_0\mu^\epsilon}\left[1-(1+\epsilon)\frac{\Sigma_0}{m_0+\Sigma}\right] \\ &= -\frac{1}{g_0}\frac{\epsilon(\Sigma+m_0)-(1+\epsilon)m_0}{m_0+\Sigma}. \end{aligned} \tag{20.85}$$

From this we deduce the stability regions for negative and positive g_0.

Let us renormalize the effective potential (20.19). Introducing the sum $\Sigma^{\rm tot} \equiv m_0 + \Sigma$, whose equilibrium value $\Sigma^{\rm tot}_0 = m_0 + \Sigma_0$ is the total finite fermion mass M. Then

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}\left[\frac{\Sigma^{{\rm tot}\,2} - 2\Sigma^{\rm tot}m_0 + m_0^2}{g_0\mu^\epsilon} - b_\epsilon\left(\frac{\Sigma^{\rm tot}}{\mu}\right)^{2+\epsilon}\mu^2\right]. \tag{20.86}$$

Here we renormalize the coupling again using Eq. (20.22). The term $2\Sigma^{\rm tot}m_0/g_0\mu^\epsilon$ is made finite by defining the renormalized mass as

$$\frac{m_0}{g_0\mu^\epsilon} = \frac{m}{g}, \tag{20.87}$$

i.e.,

$$\frac{m_0}{m} = \frac{g_0\mu^\epsilon}{g} = 1 - g_0\mu^\epsilon b_\epsilon = (1+gb_\epsilon)^{-1}. \tag{20.88}$$

The term $m_0^2/g_0\mu^\epsilon$ in (20.86) is not finite for $\epsilon \to 0$, It needs a trivial additive renormalization of the vacuum energy. Assuming that this has been supplied, we find the renormalized potential [compare (20.24)]

$$\frac{1}{N}v(\Sigma) = \frac{\mu^\epsilon}{2}\left\{\frac{(\Sigma^{\rm tot} - m)^2}{g} - b_\epsilon\Sigma^{{\rm tot}\,2}\left[\left(\frac{\Sigma^{\rm tot}}{\mu}\right)^\epsilon - 1\right]\right\}, \tag{20.89}$$

in which g and m depend on μ. The renormalized gap equation becomes

$$1 = gb_\epsilon\left[\left(1+\frac{\epsilon}{2}\right)\left(\frac{M}{\mu}\right)^\epsilon - 1\right]\frac{M}{M-m}, \tag{20.90}$$

where $\Sigma^{\rm tot}_0$ has been replaced by the fermion mass M. At $\Sigma^{\rm tot}_0 = M$, the effective potential has the value

$$\frac{1}{N}v(\Sigma) \;=\; \frac{\mu^\epsilon}{2}b_\epsilon\left[\frac{m(m-\Sigma^{\rm tot})}{g} + b_\epsilon\Sigma^{{\rm tot}\,2}\frac{\epsilon}{2+\epsilon}\right]. \tag{20.91}$$

Note that the potentials (20.24) and (20.89) for the massless and the massive models differ by a term

$$\Delta v(\Sigma) = \frac{\mu^\epsilon}{2}\frac{(\Sigma^{\rm tot} - m)^2}{g}. \tag{20.92}$$

20.6 Pairing Model and Dynamically Generated Goldstone Bosons

The model discussed in the last section is somewhat uninteresting, since the symmetry which is broken is discrete. It is instructive to consider a slightly modified situation in which there is a spontaneous breakdown of a continuous symmetry.

From the Nambu-Goldstone theorem we then expect the occurence of a massless particle. Again we consider N fields ψ_a in $D = 2 + \epsilon$ dimensions, but now we take the Lagrangian to be

$$\mathcal{L} = \bar{\psi}_a \left(i\partial\!\!\!/ - m_0 \right) \psi_a + \frac{g_0}{2N} \left(\bar{\psi}_a C \bar{\psi}_a^T \right) \left(\psi_b^T C \psi_b \right). \tag{20.93}$$

Here C is the matrix of charge conjugation which is defined by [recall (3.541)]

$$C \gamma^\mu C^{-1} = -\gamma^{\mu T}. \tag{20.94}$$

In two dimensions, where the γ-matrices have the explicit form (20.34), we may use $C = \gamma^1$:

$$C = \gamma^1 = -i\sigma^2. \tag{20.95}$$

It is the same matrix which was introduced in the four-dimensional discussion in Eq. (3.543) as the 2 × 2-submatrix c of the 4 × 4 charge conjugation matrix C.

Due to the antisymmetry of C, we have

$$\left(\bar{\psi}_a C \bar{\psi}_a^T \right)^\dagger = \psi_a^T C \psi_a. \tag{20.96}$$

As a consequence, the interaction potential in (20.93) is negative for $g_0 < 0$, amounting to an attractive potential.

Now we introduce a collective field by adding to $\mathcal{L}$ the term

$$\frac{N}{2g_0} \left| \Delta - \frac{g_0}{N} \psi_b^T C \psi_b \right|^2 ,$$

leading to the partition function

$$Z[\eta, \bar{\eta}] = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}\Delta \tag{20.97}$$
$$\times \exp \left\{ i \int d^D x \left[\bar{\psi}_a (i\partial\!\!\!/ - m_0) \psi_a + \frac{1}{2} \left(\Delta^\dagger \psi_a^T C \psi_a + \text{c.c.} \right) + \bar{\psi}\eta + \bar{\eta}\psi - \frac{N}{2g_0} |\Delta|^2 \right] \right\}.$$

In order to integrate out the Fermi fields, we rewrite the free part of Lagrangian in the matrix form

$$\frac{1}{2} \left(\psi^T C, \bar{\psi} \right) \begin{pmatrix} 0 & i\partial\!\!\!/ - m_0 \\ i\partial\!\!\!/ - m_0 & 0 \end{pmatrix} \begin{pmatrix} \psi \\ C\bar{\psi}^T , \end{pmatrix} \tag{20.98}$$

which is the same as $\bar{\psi} \left(i\partial\!\!\!/ - m_0 \right) \psi$ since

$$\begin{aligned} \psi^T C C \bar{\psi}^T &= -\psi^T \bar{\psi}^T = \bar{\psi}\psi, \\ \psi^T C \overset{\leftrightarrow}{\partial\!\!\!/} C \bar{\psi}^T &= \psi^T \overset{\leftrightarrow}{\partial\!\!\!/}{}^T \bar{\psi}^T = \bar{\psi} \partial\!\!\!/ \psi. \end{aligned} \tag{20.99}$$

But then the interaction with Δ can be combined with (20.81) in the form

$$\frac{1}{2}\phi_i^T\, iG_\Delta^{-1}\phi \tag{20.100}$$

where

$$\phi \equiv \left(\begin{array}{c}\psi\\ C\bar\psi^T\end{array}\right),\quad \phi^T \equiv \left(\psi^T,\bar\psi C^{-1}\right) \tag{20.101}$$

denotes the doubled fermion field and

$$iG_\Delta^{-1} = \left(\begin{array}{cc}C & 0\\ 0 & C\end{array}\right)\left(\begin{array}{cc}\Delta^\dagger & i\partial\!\!\!/ - m_0\\ i\partial\!\!\!/ - m_0 & \Delta\end{array}\right) \tag{20.102}$$

is the inverse propagator in the presence of the external field Δ. Observe that ϕ is a quasi-real field since ϕ^* related to ϕ by the similarity transformation

$$\phi^* = \left(\begin{array}{c}\psi^*\\ C\bar\psi^{T*}\end{array}\right)=\left(\begin{array}{cc}0 & C\gamma^0\\ C\gamma^0 & 0\end{array}\right)\left(\begin{array}{c}\psi\\ C\bar\psi^T\end{array}\right)=\left(\begin{array}{cc}0 & C\gamma^0\\ C\gamma^0 & 0\end{array}\right)\phi. \tag{20.103}$$

For a quasi-real field, G_Δ^{-1} must be an antisymmetric matrix in the combined spinor and functional space, and this can easily be verified:

$$\begin{aligned}\left(\begin{array}{cc}C\Delta^\dagger & C(\partial\!\!\!/ - m_0)\\ C(\partial\!\!\!/ - m_0) & C\Delta\end{array}\right)^T &= \left(\begin{array}{cc}C^T\Delta^\dagger & (\partial\!\!\!/^T - m_0)C^T\\ (\partial\!\!\!/^T - m_0)C^T & C^T\Delta\end{array}\right)\\ &= -\left(\begin{array}{cc}C\Delta^\dagger & C(\partial\!\!\!/ - m_0)\\ C(\partial\!\!\!/ - m_0) & C\Delta\end{array}\right)\end{aligned} \tag{20.104}$$

since$C\partial\!\!\!/^TC^{-1} = \gamma^\mu\partial_\mu^T = -\partial\!\!\!/$, where the transposion applies to the combined space, which is the origin of the negative sign with respect to the relation $C\gamma^{\mu^T}C^{-1} = -\gamma^\mu$ of Eq. (20.94). In spinor space, partial integration makes the derivative ∂ equivalent to the manifestly antisymmetric functional matrix $\frac{1}{2}(\overrightarrow{\partial} - \overleftarrow{\partial})$. In momentum space, the kinetic part of $iG_\Delta^{-1}(p',p) = \delta^{(2)}(p'+p)iG_\Delta^{-1}(p)$ is antidiagonal in momentum space, satisfying $G_\Delta^T(p,p') = -G_\Delta(p,p')$, since $\delta^{(D)}(p'+p)p$ is an antisymmetric functional matrix. This is necessary to have a nonzero kinetic part in the fermionic Lagrangian, which reads in terms of the quasi-real field $\phi(p)$:

$$\int d^Dp'd^Dp\,\phi(p')\,iG_\Delta^{-1}(p',p)\phi(p) = \int d^Dp\,\phi(-p)\,iG_\Delta^{-1}(p)\phi(p). \tag{20.105}$$

We can now perform the functional integral over the fermion fields according to the rule (10.95), leading to

$$Z[j] = \int \mathcal{D}\Delta\mathcal{D}\Delta^\dagger e^{iN\mathcal{A}[\Delta]+\frac{1}{2}j_a^TG_\Delta j_a}, \tag{20.106}$$

where $\mathcal{A}[\Delta]$ is the collective action

$$\mathcal{A}[\Delta] = -\frac{1}{2g_0}\int d^Dx\,|\Delta|^2 - \frac{i}{2}\mathrm{Tr}\,\log iG_\Delta^{-1}, \tag{20.107}$$

and j_a is the doubled version of the external source in analogy to (20.86)

$$j = \begin{pmatrix} \bar{\eta}^T \\ C^{-1}\eta \end{pmatrix}. \tag{20.108}$$

This is chosen so that

$$\bar{\psi}\eta + \bar{\eta}\psi = \frac{1}{2}\left(j^T\phi - \phi^T j\right), \tag{20.109}$$

and a quadratic completion gives

$$\frac{1}{2}\phi^T iG_\Delta^{-1}\phi + \frac{1}{2}(j^T\phi - \phi^T j) = \frac{1}{2}(\phi^T + j^T iG_\Delta^T) iG_\Delta^{-1}(\phi + iG_\Delta j) - \frac{i}{2}j^T G_\Delta j. \tag{20.110}$$

Note the sign change in front of $\frac{1}{2}j^T G_\Delta j$ in Eq. (20.106) with respect to the Bose case, in accordance with the negative relative sign of the source term $\frac{1}{2}(j^T\phi - \phi^T j)$.

In the limit $N \to \infty$ we obtain from (20.107) the effective action

$$\frac{1}{N}\Gamma[\Delta, \Psi] = \frac{1}{2g_0}|\Delta|^2 - \frac{i}{2}\mathrm{Tr}\,\log iG_\Delta^{-1} + \frac{1}{2N}\Phi_a^T iG_\Delta^{-1}\Phi_a \tag{20.111}$$

in the same way as in the last chapter for the simpler model with a real σ-field.

The ground state has $\Phi = 0$, whereas $\Delta = \Delta_0$ satisfies the gap equation

$$\frac{\Delta_0}{g_0} = -\frac{1}{2}\mathrm{tr}\,G_{\Delta_0}\begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix}, \tag{20.112}$$

where we may assume Δ_0 to be real, as we shall show later.

As before, we shall consider first the case of zero initial mass m_0. Then the Green's function is inverted as follows

$$G_{\Delta_0}(x,y) = \int \frac{d^Dp}{(2\pi)^D} e^{-ip(x-y)} \frac{i}{p^2 - \Delta_0} \begin{pmatrix} -\Delta_0 & \not{p} \\ \not{p} & -\Delta_0 \end{pmatrix} \begin{pmatrix} C^{-1} & 0 \\ 0 & C^{-1} \end{pmatrix}, \tag{20.113}$$

as we can verify by multiplying with (20.102). Thus the gap equation (20.112) is simply

$$\frac{1}{g_0} = 2^{D/2}\int \frac{d^Dp}{(2\pi)^D} \frac{1}{p^2 + M^2}, \tag{20.114}$$

where we have introduced the notation

$$M \equiv \Delta_0, \tag{20.115}$$

to indicate the significance of Δ_0 as a spontaneously generated fermion mass. Also, we have taken the trace in Dirac space to be $2^{D/2}$ in D dimensions.

The integral in (20.113) can be performed just as before and we find

$$\frac{1}{g_0\mu^\epsilon} = -b_\epsilon \frac{D}{\epsilon}\left(\frac{M}{\mu}\right)^\epsilon . \tag{20.116}$$

The effective potential is now for $\Phi_a = 0$:

$$\frac{1}{N}v(\Delta) = \frac{1}{2g_0}|\Delta|^2 + \frac{i}{2}\int \frac{d^Dp}{(2\pi)^D}\log\begin{pmatrix} \Delta^\dagger & \not{p} \\ \not{p} & \Delta \end{pmatrix}, \tag{20.117}$$

such that we obtain, after a Wick rotation,

$$\frac{1}{N}v(\Delta) = \frac{1}{g_0}|\Delta|^2 - \frac{1}{2}2^{D/2}\int \frac{d^Dp_E}{(2\pi)^D}\log\left(p_E^2 + |\Delta|^2\right).$$

Performing the integral gives

$$\begin{aligned} \frac{1}{N}v(\Delta) &= \frac{1}{2g_0}|\Delta|^2 - \frac{1}{2}2^{D/2-1}S_D\Gamma(D/2)\Gamma\left(1-\frac{D}{2}\right)\frac{2}{D}|\Delta|^D \\ &= \frac{\mu^\epsilon}{2}\left[\frac{|\Delta|^2}{g_0\mu^\epsilon} - b_\epsilon\left(\frac{|\Delta|}{\mu}\right)^{2+\epsilon}\mu^2\right], \end{aligned} \tag{20.118}$$

from which the gap equation (20.116) can again be recovered by differentiation. Stability is insured for $g_0 < 0$, i.e., for attractive interactions. For $\Delta_0 = 0$, only the trivial solution $\Delta_0 = 0$ is stable.

For $\Delta_0 \neq 0$, we may use (20.116) and express the potential in terms of M rather than the bare coupling constant g_0 as

$$\frac{1}{N}v(\Delta) = \frac{M^\epsilon}{2}b_\epsilon|\Delta|^2\left[\frac{D}{2} - \left(\frac{|\Delta|}{M}\right)^\epsilon\right]. \tag{20.119}$$

As before in (20.22), $v(\Delta)$ can be expressed in terms of the renormalized coupling

$$\frac{1}{g_0\mu^\epsilon} - b_\epsilon = \frac{1}{g}, \tag{20.120}$$

in the alternative form

$$\frac{1}{N}v(\Delta) = \frac{\mu^\epsilon}{2}\left\{\frac{|\Delta|^2}{g} + b_\epsilon\left[1 - \left(\frac{|\Delta|}{\mu}\right)^{D-2}\right]|\Delta|^2\right\}. \tag{20.121}$$

From either expression, we find in the limit $\epsilon \to 0$:

$$\begin{aligned} \frac{1}{N}v(\Delta) &= \frac{1}{2\pi}\left(\log\frac{|\Delta|}{M} - \frac{1}{2}\right)|\Delta|^2 \\ &= \frac{1}{2}\left[\frac{|\Delta|^2}{g} + \frac{1}{\pi}|\Delta|^2\log\frac{|\Delta|}{\mu}\right], \end{aligned} \tag{20.122}$$

in analogy to (20.23) and (20.45) .

Let us now study the propagator of the complete Δ-field. For small deviations $\Delta' \equiv \Delta - \Delta_0$ from the ground state value of Δ, we find from (20.111) the quadratic term

$$\frac{1}{N}\delta^2\Gamma = -\frac{1}{2}\left\{\int d^Dx\,\frac{|\Delta|^2}{g_0} + \frac{i}{2}\mathrm{Tr}\left[\begin{pmatrix} \Delta'^\dagger & \\ & \Delta' \end{pmatrix} G_M \begin{pmatrix} \Delta'^\dagger & \\ & \Delta' \end{pmatrix} G_M\right]\right\}. \quad (20.123)$$

In momentum space, the trace term may be written more explicitly as

$$\frac{i}{2}\left\{M^2\left[\Delta'(q)\Delta'(-q) + \Delta'^*(q)\Delta'^*(-q)\right]2^{D/2}\int\frac{d^Dk}{(2\pi)^D}\frac{i}{k^2-M^2}\frac{i}{(k-q)^2-M^2}\right.$$
$$\left.+\left[\Delta'(q)\Delta'^*(-q) + \Delta'(-q)\Delta'^*(q)\right]\int\frac{d^Dk}{(2\pi)^D}\frac{i}{k^2-M^2}\frac{i}{(k-q)^2-M^2}\mathrm{tr}\left[\not{k}\,(\not{k}-\not{q}\,)\right]\right\}.$$

In a Wick-rotated form, this becomes

$$\frac{1}{2}\left\{M^2\left[\Delta'(q)\Delta'(-q) + \Delta'^*(q)\Delta'^*(-q)\right]\tilde{\Pi}(q_E^2/M^2)\right.$$
$$\left.+\left[\Delta'(q)\Delta'^*(-q) + \Delta'(-q)\Delta'^*(q)\right]\left[\Pi(q_E^2/M^2) - M^2\tilde{\Pi}(q_E^2/M^2)\right]\right\}, \quad (20.124)$$

where $\Pi(q_E^2/M^2)$ is the previous self-energy (20.49) calculated in (20.55). The slightly simpler quantity $\tilde{\Pi}\left(q_E^2/M^2\right)$ stands for

$$\tilde{\Pi}\left(q_E^2/M^2\right) = i\,2^{D/2}\int\frac{d^Dk}{(2\pi)^D}\frac{i}{k^2-M^2}\frac{i}{(k-q)^2-M^2},$$

and is calculated as follows:

$$\begin{aligned}\tilde{\Pi}\left(q_E^2/M^2\right) &= 2^{D/2}\int\frac{d^Dk_E}{(2\pi)^D}\int_0^1 dx\,\frac{1}{\left[k_E^2+q_E^2x(1-x)+M^2\right]^2}\\ &= 2^{D/2}S_D\frac{1}{2}\Gamma(D/2)\Gamma(2-D/2)\int_0^1 dx\left[q_E^2x(1-x)+M^2\right]^{D/2-2}\\ &= -\frac{D}{2}b_\epsilon(1-D/2)\int_0^1 dx\left[q_E^2x(1-x)+M^2\right]^{D/2-2}.\end{aligned}$$

As a result, the action for the quadratic deviations from Δ_0 can be written as

$$\frac{1}{N}\delta^2\Gamma = -\frac{V}{4}\int\frac{d^Dq}{(2\pi)^D}\left\{\left(\frac{1}{g_0}+A\right)\left[\Delta'(q)\Delta'^*(-q)+\Delta'(-q)\Delta'^*(q)\right]\right.$$
$$\left.+B\;\left[\Delta'(q)\Delta'(-q)+\Delta'^*(q)\Delta'^*(-q)\right]\right\}, \quad (20.125)$$

with the coefficients

$$\begin{aligned}A &= \Pi(q_E^2/M^2) - \tilde{\Pi}(q_E^2/M^2)\\ &= -\frac{D}{2}b_\epsilon M^\epsilon\left[(D-1)J_1^\epsilon(q_E^2/M^2) + (1-D/2)J_2^\epsilon(q_E^2/M^2)\right], \quad (20.126)\\ B &= \tilde{\Pi}(q_E^2/M^2)\\ &= \frac{D}{2}b_\epsilon(1-D/2)M^\epsilon J_2^\epsilon(q_E^2/M^2), \quad (20.127)\end{aligned}$$

and the integrals

$$J_1^\epsilon(z)=\int_0^1 dx\,[zx(1-x)+1]^{D/2-1}\,,\quad J_2^\epsilon(z)=\int_0^1 dx\,[zx(1-x)+1]^{D/2-2}\,. \tag{20.128}$$

Thus the propagators of real and imaginary parts of the field Δ' are

$$G_{\Delta'_{\rm re}\Delta'_{\rm re}} = -\frac{i}{N}\frac{1}{g_0^{-1}+A+B} \tag{20.129}$$

$$G_{\Delta'_{\rm im}\Delta'_{\rm im}} = -\frac{i}{N}\frac{1}{g_0^{-1}+A-B} \tag{20.130}$$

and for the complex fields Δ', $\Delta'^\dagger$:

$$G_{\Delta'^\dagger\Delta'^\dagger} = -2\frac{i}{N}\frac{1}{\left(g_0^{-1}+A\right)^2-B^2}(-B), \tag{20.131}$$

$$G_{\Delta'\Delta'^\dagger} = -2\frac{i}{N}\frac{1}{\left(g_0^{-1}+A\right)^2-B^2}\left(g_0^{-1}+A\right). \tag{20.132}$$

The expressions (20.129)–(20.132) can be made finite by using the gap equation (20.116). The term involving $1/g_0$,

$$\frac{1}{g_0}+A=\frac{D}{2}b_\epsilon M^\epsilon\left\{\left[1-(D-1)J_1^\epsilon\left(q_E^2/M^2\right)\right]-(1-D/2)\,J_2^\epsilon\left(q_E^2/M^2\right)\right\}, \tag{20.133}$$

depends then only on the parameter M, and remains finite for $\epsilon\to 0$, where it becomes

$$\frac{1}{g_0}+A\to\frac{1}{2\pi}\left\{\left[J(q_E^2/M^2)+2\right]-J_2^0(q_E^2/M^2)\right\}, \tag{20.134}$$

where $J(z)=2dJ_2^\epsilon(z)/d\epsilon|_{\epsilon=0}$ is the function (20.61). The function B needs no renormalization, and has the $\epsilon\to 0$ -limit

$$B\underset{\epsilon\to 0}{\longrightarrow}\frac{1}{2\pi}J_2^0(q_E^2/M^2). \tag{20.135}$$

We now observe that there is a zero mass excitation in the imaginary part of the Δ'-field, the component of Δ which points orthogonal to the real ground state value $\Delta_0=M$. To show this we consider the denominator of the propagator (20.130):

$$\frac{1}{g_0}+A-B=\frac{D}{2}b_\epsilon M^\epsilon\left\{\left[1-(D-1)J_1^\epsilon(q_E^2/M^2)\right]-(2-D)J_2^\epsilon(q_E^2/M^2)\right\}. \tag{20.136}$$

By expanding in powers of $z \equiv q_E^2/M^2$,

$$\begin{aligned} J_1^\epsilon &\sim 1+\frac{D-2}{12}z+\mathcal{O}(z^2), \\ J_2^\epsilon &\sim 1+\frac{D-4}{12}z+\mathcal{O}(z^2), \end{aligned} \tag{20.137}$$

we find for small momenta

$$\begin{aligned} \frac{1}{g_0}+A-B &= \frac{D}{2}b_\epsilon M^\epsilon\left\{\left[1-(D-1)\left(1+\frac{D-2}{12}z\right)\right]-(2-D)\left(1+\frac{D-4}{12}z\right)\right\}+\mathcal{O}(z^2) \\ &= -\frac{D}{2}b_\epsilon M^\epsilon\frac{D-2}{4}z+\mathcal{O}(z^2), \end{aligned} \tag{20.138}$$

such that the propagator of (20.130) becomes, expressed in terms of Minkowski square momentum $q^2=-q_E^2$,

$$G_{\Delta'_{\rm im}\Delta'_{\rm im}}=-\frac{1}{N}\frac{2}{D(D-2)b_\epsilon}4M^{2-\epsilon}\frac{i}{q^2}+\text{regular part at } q^2=0. \tag{20.139}$$

Since $b_\varepsilon<0$ for $D>2$, the residue is positive

$$\text{Res } G_{\Delta'_{\rm im}\Delta'_{\rm im}}\approx-\frac{1}{N}\frac{2}{D(D-2)b_\epsilon}4M^{2-\epsilon}\to\frac{4\pi}{N}M^2, \tag{20.140}$$

such that the propagator exhibits a proper particle pole at $q^2=0$. The positive sign is necessary for a positive norm of the corresponding particle state in the Hilbert space.

In the limit $\epsilon\to0$, expression (20.136) becomes

$$\frac{1}{g_0}+A-B\underset{\epsilon\to0}{\to}\frac{1}{2\pi}[J(z)+2-2J_2^0(z)]. \tag{20.141}$$

The integral $J(z)$ was calculated in Eq. (20.61). For the integral $J_2^0(z)$, we find by a similar calculation

$$J_2^0(z)=\frac{2\theta}{\sinh 2\theta}=\frac{\theta\coth\theta}{\cosh^2\theta}=\frac{2}{z+4}[J(z)+2], \tag{20.142}$$

such that we obtain in Minkowski space with with $z\equiv q_E^2/M^2=-q^2/M^2$:

$$\begin{aligned} G_{\Delta'_{\rm im}\Delta'_{\rm im}} &= \frac{i}{N}2\pi\frac{1}{2\theta\tanh\theta} \\ &= \frac{i}{N}2\pi\frac{4M^2-q^2}{q^2}\frac{1}{J(-q^2/M^2)+2}. \end{aligned} \tag{20.143}$$

The real part of the fluctating field Δ' has for $\epsilon\to0$ the propagator

$$G_{\Delta'_{\rm re}\Delta'_{\rm re}}=-\frac{i}{N}2\pi\frac{1}{J(-q^2/M^2)+2}. \tag{20.144}$$

20.7 Spontanously Broken Symmetry

When finding the pole at $q^2 = 0$, we have said that this particle was a Nambu-Goldstone boson. In order to justify this association, we have to exhibit the continuous symmetry which has been spontaneously broken by the ground state solution. Looking back at the original Lagrangian (20.93), we see that it is invariant under global gauge transformations

$$\begin{aligned} \psi &\rightarrow e^{i\alpha}\psi, \qquad \alpha = \text{const.} \\ \bar{\psi} &\rightarrow e^{-i\alpha}\psi. \end{aligned} \tag{20.145}$$

Similarly, the collective action (20.97) remains invariant, if the collective field Δ which is, on the average, equal to a pair of ψ-fields is transformed with twice the phase angle:

$$\Delta \rightarrow e^{2i\alpha}\Delta \tag{20.146}$$

This invariance has been used before when we chose a real ground state expectation Δ_0. Any other phase would have given the same physical result. Of course, once this phase is chosen, the invariance (20.145) is destroyed. Thus the zero-mass particle is indeed a Nambu-Goldstone particle. It corresponds to excitation whose long-wavelength limit reduces to a pure global gauge transformation.

Strictly speaking, this zero mass boson can only exist in dimensions $D > 2$, as follows from a very general theorem of Mermin, Wagner, and Coleman (see Footnote 4). Indeed, we have seen before in the Bose case that fluctuations prevent the spontaneous breakdown of a continuous symmetry, which might be resent at the mean-field level. Thus we may conclude that if fluctuations were included in the collective field, the theory would also exhibit this general feature in two space-time dimensions. In the limit $N \rightarrow \infty$ there are no fluctuations in Δ. Thus Coleman's theorem should be satisfied after including all $1/N$ corrections. Things are more subtle, however. In two dimensios, there is a critical coupling strength where a quasi-ordered state exists. This will be discussed in Subsection 20.8.

The physical interpretation of the field Δ is the following: Due to the attraction for $g_0 < 0$, the fermions form bound state pairs, called, *Cooper pairs*, which are bosons and can form a condensate, just as before the bosonic ϕ fields in ϕ^4 theory. In fact, the effective potential for the Δ-field looks qualitatively very similar to that of the bosonic potential $v(\Delta)$ of the O(N)-symmetric theory for negative m^2. The origin is unstable and there is a new minimum at $\Delta_0 \neq 0$ with an arbitrary phase [see (20.100) with $m_0 = 0$]. Just as in the previous model with an interaction $(g_0/2N)\left(\bar{\psi}_a\psi_a\right)^2$, the opposite sign $g_0 > 0$ does not lead to a spontaneous symmetry breakdown, and massless fermions remain massless.

Finally we must justify why we have called the vacuum expectation $\Delta_0 = M$ the spontanoeusly generated fermion mass. Looking back at the collective effective action (20.111), we see that the Δ_0 fields appear in the form

$$\overline{\Psi} i\partial\!\!\!/ \Psi + \frac{1}{2}M\left(\Psi^T C\Psi + \overline{\Psi} C\overline{\Psi}^T\right) = \frac{1}{2}\left(\Psi^T C, \overline{\Psi}\right)\begin{pmatrix} M & i\partial\!\!\!/ \\ i\partial\!\!\!/ & M \end{pmatrix}\begin{pmatrix} \Psi \\ C\overline{\Psi}^T \end{pmatrix}. \tag{20.147}$$

There is a simple transformation which brings this to the canonical Dirac form. With the two-dimensional γ^5-matrix (20.36), we see that

$$\Psi' = \frac{1-\gamma_5}{2}\Psi + \frac{1+\gamma_5}{2}C\overline{\Psi}^T, \qquad \bar{\Psi}' = \overline{\Psi}\frac{1+\gamma_5}{2} + \Psi^T C\frac{1-\gamma_5}{2}, \tag{20.148}$$

and hence

$$\overline{\Psi}'\Psi' = \frac{1}{2}\left(\Psi^T C\Psi + \overline{\Psi}C\overline{\Psi}^T\right) - \frac{1}{2}\left(\Psi^T C\gamma_5\Psi - \overline{\Psi}\gamma^5 C\overline{\Psi}^T\right), \tag{20.149}$$

where we have used the projection property

$$P_\pm^2 = P_\pm \tag{20.150}$$

of the chiral projection matrix

$$P_\pm \equiv \frac{1\pm\gamma_5}{2}, \tag{20.151}$$

and the fact that

$$\gamma_\mu P_\pm = P_\mp \gamma\mu, \tag{20.152}$$

which implies that

$$P_\pm\gamma_0 P_\pm = 0, \qquad P_\pm\gamma_0 P_\mp = \gamma_0, \tag{20.153}$$

But the γ_5-terms in (20.149) vanish due to the relations

$$C\gamma_5^T C^{-1} = C\left(\gamma^0\gamma^1\right)^T C^{-1} = -\gamma^0\gamma^1 = -\gamma_5. \tag{20.154}$$

Thus the mass term in Eq. (20.147) becomes simply $M\overline{\Psi}'\Psi'$.

The gradient term in (20.147) is invariant under the transformation (20.148):

$$\overline{\Psi}' i\partial\!\!\!/\, \Psi' = \overline{\Psi} i\partial\!\!\!/\, \Psi. \tag{20.155}$$

This follows again from (20.152), imlying here that

$$P_\pm\gamma_0\gamma_\mu P_\pm = \gamma_0\gamma_\mu, \qquad P_\pm\gamma_0\gamma_\mu P_\mp = 0, \tag{20.156}$$

In this context it should be mentioned that the whole model could have been written in terms of ψ'-fields defined in terms of ψ-fields as in (20.148) from the outset. If we supplement the relation (20.149) by

$$\overline{\Psi}'\gamma_5\Psi' = -\frac{1}{2}\left(\Psi^T C\Psi - \overline{\Psi}C\overline{\Psi}^T\right) + \frac{1}{2}\left(\Psi^T C\gamma_5\Psi + \overline{\Psi}\gamma_5 C\Psi^T\right), \tag{20.157}$$

where the second parenthesis is again zero, we see that the fermion field part in the effective action (20.97) can be written for zero sources and mass as

$$\begin{aligned}\overline{\Psi}_a i\partial\!\!\!/\, \Psi_a &+ \frac{1}{2}\Delta_{\rm re}\left(\Psi_a^T C\Psi_a + \overline{\Psi}_a C\overline{\Psi}_a^T\right) - \frac{i}{2}\Delta_{\rm im}\left(\Psi_a^T C\Psi_a - \overline{\Psi}_a C\overline{\Psi}_a^T\right)\\ &= \overline{\Psi}'_a\left(i\partial\!\!\!/ - \sigma - i\pi\gamma_5\right)\Psi'_a - \frac{N}{2g_0}(\sigma^2+\pi^2),\end{aligned} \tag{20.158}$$

where we have identified

$$\sigma \equiv -\Delta_{\rm re}, \qquad \pi = -\Delta_{\rm im}. \tag{20.159}$$

The invariance under global gauge transformation (20.145) becomes, in terms of Ψ'-fields, an invariance under the transformation

$$\Psi' \equiv \begin{pmatrix} -\Psi_1^* \\ \Psi_2 \end{pmatrix} \rightarrow \begin{pmatrix} -e^{i\alpha}\Psi_1^* \\ e^{-i\alpha}\Psi_2 \end{pmatrix}, \tag{20.160}$$

$$= \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \Psi' = e^{i\alpha\gamma_5}\Psi'. \tag{20.161}$$

Such transformations involving γ_5 are referred to as *chiral transformations* , and play an important role in theoris of weak interactions (See Chapter 24). Under the chiral transformation, $\bar\Psi'\Psi'$ and $\bar\Psi' i\gamma_5\Psi$ behave like a vector in a plane

$$\begin{aligned} \bar\Psi'\Psi' &\rightarrow \bar\Psi' e^{2i\alpha\gamma_5}\Psi' = \cos 2\alpha \bar\Psi'\Psi' + \sin 2\alpha \bar\Psi' i\gamma_5\Psi' \\ \bar\Psi' i\gamma_5\Psi' &\rightarrow \bar\Psi' e^{i\alpha\gamma_5}\gamma_5 e^{i\alpha\gamma_5}\Psi' = -\sin 2\alpha \bar\Psi'\Psi' + \cos 2\alpha \bar\Psi' i\gamma_5\Psi'. \end{aligned} \tag{20.162}$$

Thus, the transformation (20.146) becomes with (20.149) and (20.157):

$$\begin{pmatrix} \sigma \\ \pi \end{pmatrix} \rightarrow \begin{pmatrix} \sigma' \\ \pi' \end{pmatrix} = \begin{pmatrix} \cos 2\alpha & \sin 2\alpha \\ -\sin 2\alpha & \cos 2\alpha \end{pmatrix} \begin{pmatrix} \sigma \\ \pi \end{pmatrix}, \tag{20.163}$$

which lesves the tranformed effective action (20.158) chirally invariant.

The ground state breaks chiral invariance since σ acquires an expectation value $\sigma_0 = M$. The Nambu-Goldstone boson generated by this phase transition is the massless field π. It is for this reason that chiral invariance is believed to be an important principle of strong interactions among elementary particles. There is a particle in nature, the pion, whose mass is a particle in nature, the pion, whose electrically neutral version has a mass of 135 MeV, and lies much lower than any other strongly interacting particle. One therefore interpretes the pion as an almost Nambu-Goldstone particle of the underlying Lagrangian. It was really in this context that Nambu initiated the study of chiral symmetry in particle physics.

Finally, let us remark that the inclusion of an initial fermion mass $m_0 \neq 0$ is possible but will not be done here, since it merely makes the discussion more involved while adding little to the understanding of the model.

In $D = 2+\epsilon$ dimensions, the model with the Lagrangian

$$\mathcal{L} = \bar\psi_a \left(i\not\partial - m_0 - \sigma - i\pi\gamma_5\right)\psi_a + \frac{g_0}{2N}\left[\left(\bar\psi_a\psi_a\right)^2 + \left(\bar\psi_a i\gamma_5\psi_a\right)^2\right], \tag{20.164}$$

which after the introduction of collective fields $\sigma$and π as in Eq. (20.6) corresponds to a Lagrangian

$$\mathcal{L} = \bar\psi_a \left(i\not\partial - m_0 - \sigma - i\pi\gamma_5\right)\psi_a + \frac{N}{2g_0}\left(\sigma^2 + \pi^2\right), \tag{20.165}$$

and thus to the effective action (20.158), is called the *chiral Gross-Neveu model.*

20.8 Relation between Pairing and Gross-Neveu Model

Both models discussed in the last chapter showed spontaneous mass generation in the limit of $N \to \infty$ only for one sign of the bare coupling constant: the Gross-Neveu model (20.6) only for an interaction

$$\frac{g_0}{N}\left(\bar{\psi}_a\psi_a\right)^2, \qquad \text{with } g_0 < 0, \tag{20.166}$$

and the pairing model (20.97) only for

$$\frac{g_0}{N}\psi_a^T C\psi_a\bar{\psi}_b C\bar{\psi}_b^T, \qquad \text{with } g_0 < 0. \tag{20.167}$$

For the forces between the fermions described by the fields, the latter case implies attraction, the first repulsion. In either case, the opposite sign of g_0 leaves the fermions massless for $N \to \infty$.

These exactly soluble models may be an idealized limiting descriptions of two phases of the not exactly solvable $N = 1$ model

$$\mathcal{L} = \bar{\psi}i\partial\!\!\!/\,\psi + \frac{g_0}{2}\left(\bar{\psi}\psi\right)^2 \tag{20.168}$$

for $D > 2$.[5] As before, we can certainly introduce a collective field σ as in the partition function (20.6). But for $N = 1$, the field σ will fluctuate strongly, such that the phase properties of the model cannot be derived in this way. Suppose now that fluctuations do not completely destroy the fact that for $g_0 < 0$ there is a solution in which a mass is generated spontaneously, i.e., that the $N \to \infty$ limit gives at least a qualitatively correct description of the system for $g_0 < 0$.

Then we would tend to believe that also the $N = 1$ version of the pairing model

$$\mathcal{L} = \bar{\psi}i\partial\!\!\!/\,\psi + \frac{g_0}{2}\psi^T C\psi\bar{\psi}C\bar{\psi}^T \tag{20.169}$$

should have a solution for $g_0 < 0$ which resembles that of the $N \to \infty$ limit, i.e., in which there are massive fermions. But the associated Cooper pair fields would then describe bound states which carry massless Nambu-Goldstone bosons.

The interesting observation is no that these solutions of the two models are two different phases of one and the same model model. The point is that the interactions in the Lagrangians (20.168) and (20.169) are really identical, apart from an opposite sign of the coupling constant, and a factor two. This follows directly by rewriting the interactions in terms of spin up and spin down components of the field $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$. For the interaction in (20.168), we obtain

$$(\bar{\psi}\psi)^2 \;=\; (\psi_2^*\psi_1 + \psi_1^*\psi_2)^2 = 2\psi_2^*\psi_1\psi_1^*\psi_2, \tag{20.170}$$

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[5] I. Ojima and R. Fukuda, Progr. Theor. Phys. *57*, 1720 (1977)

We have omitted terms containing squares of the fields $\psi_1^2 = \psi_2^2$ and their conjugates, since these vanish for Grassmann variables. Proceeding similarly with the interaction in (20.169), we obtain

$$\begin{aligned} |\psi^T C\psi|^2 &= |-\psi_1\psi_2+\psi_2\psi_1|^2 = |2\psi_2\psi_1|^2 \\ &= 4(\psi_2\psi_1)^*\psi_2\psi_1 = 4\psi_1^*\psi_2^*\psi_2\psi_1 = -4\psi_2^*\psi_1\psi_1^*\psi_2, \end{aligned} \tag{20.171}$$

such that, indeed,

$$\left(\bar\psi\psi\right)^2 = -\frac{1}{2}|\psi^T C\psi|^2. \tag{20.172}$$

Thus we expect the following two phases for the $N=1$ -model: for $g_0 < 0$ or $g > g^*$, a phase with massive fermions and a spontaneously broken γ_5 invariance. Here the system is symmetric under global gauge transformations. The other physe for $g_0 > 0, g < g^*$ has again massive fermions but, in addition, massless Nambu-Goldstone modes due to a spontaneously broken global gauge symmetry. Physically, the second phases will be distinguished from the first by the strong long-range fluctuations which do not exist in the first phase.

For $N \to \infty$, either of the two phases forms the only existing solution of the two models which differ by the distributes the indices over the four fermion fields in (20.166) and (20.167).

We pointed out before the analogy between the coupling constant in this model and the temperature in the euclidean formulation of the model. With this interpretation of g, the behavior of this model looks very similar to that found experimentally in thin films of ^{4}He. There is a phase transition at a certain temperature T_c. Above T_c there are only short-range correlations (the system is normal). Below there are long-range correlations (the system is super-fluid) due to Goldstone excitations of the condensate. By the Mermin-Wagner theorem discussed on page 781, there can be no Nambu-Goldstone in exactly two dimensions, but there do exist quasi-long-range fluctuations with power-like correlation functions of the type (17.98).

20.9 Comparison with O(N)-Symmetric ϕ^4-Theory

After having observed the possibility of spontaneously generating a mass in a massles theory via fluctuations we may look once more back at the scalar ϕ^4 version of the O(N) model in $D = 4-\varepsilon$ dimensions. Note the different notation for $\varepsilon \equiv 4-D$ in contrast to $\epsilon \equiv D-2$ in the other sections. In the massless case the potential is

$$v(\Phi,\lambda) = \frac{1}{2}\lambda\Phi_a^2 - \frac{N}{4g_0}\lambda^2 + \frac{1}{2}NS_D\frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}\lambda^{D/2} \tag{20.173}$$

which may be written as

$$\frac{1}{N}v(\Phi,\lambda) = \frac{1}{2N}\lambda\Phi_a^2 - \frac{1}{4g_0}\lambda^2 - \frac{b'_\varepsilon}{4}\lambda^{D/2} \tag{20.174}$$

with

$$b'_\varepsilon \equiv -\frac{2}{D}S_D\Gamma(D/2)\Gamma(1-D/2) = \frac{4}{D}S_D\frac{1}{\varepsilon} \approx \frac{1}{8\pi^2}\frac{1}{\varepsilon} \tag{20.175}$$

Note the opposite, bosonic, sign of the last term (20.173) in comparison with the fermionic equation (20.17), and the absense in b'_ε of a factor $2^{D/2-1}$ with respect to the fermionic b_ϵ in Eq. (20.20), which came from the Dirac trace in D dimensions, and a factor 1/2 caused by the linearity of the Dirac operator in p. The bosonic b'_ε is related to the bosonic constant introduced in the discussion of the nonlinear σ-model in Eq. (18.37) by $b'_\varepsilon = 4c_\epsilon/D = b'_\varepsilon$.

The two gap equations are

$$\lambda\Phi_a = 0, \tag{20.176}$$

to be solved by $\lambda = 0$ or $\phi_a = 0$. and

$$\frac{1}{N}\Phi_a^2 - \frac{1}{g_0}\lambda - b'_\varepsilon\frac{D}{4}\lambda^{D/2-1} = 0. \tag{20.177}$$

A renormalized coupling constant may be introduced by setting

$$\frac{1}{g_0\mu^{-\varepsilon}} + b'_\varepsilon = \frac{1}{g} \tag{20.178}$$

and $v(\Phi,\lambda)$ becomes

$$\frac{1}{N}v(\Phi,\lambda) = \frac{1}{2N}\lambda\Phi_a^2 - \frac{\mu^{-\varepsilon}}{4}\left\{\frac{\lambda^2}{g} + b'_\varepsilon\left[\left(\frac{\lambda}{\mu^2}\right)^{-\varepsilon/2} - 1\right]\lambda^2\right\}. \tag{20.179}$$

In the renormalized form, the different signs of the bare coupling $g_0 >$ or $g_0 < 0$ correspond to $g < g^*$ or $g > g^*$ with $g^* = b'^{-1}_\varepsilon \approx 8\pi^2\varepsilon$.

There is a O(N)-symmetric phase with $\Phi_a = 0$ and $\lambda_0 \neq 0$ for $g_0 < 0$, where the bosons acquire a mass. For $g_0 < 0$ there is only the solution $\Phi_a = 0$, $\lambda_0 = 0$ which is again a symmetric phase, but contrary to the previous one this is massless.

Both phases are stable, since the determinant of the second-derivative matrix $v_{ab}(\Phi_a, \lambda(\Phi_a^2))$ is nonnegative, where a subscript a abbreviates the dericative $\partial/\partial\Phi_a$, and $\lambda(\Phi_a^2)$ is the solution of the gap equation (20.177)

Consider, however, the excitations: In the massless phase with $g < g^*$, we calculate the propagator $G_{\Sigma'\Sigma'}$ from the quadratic variation

$$\delta^2\Gamma[\Phi,\Sigma] = \frac{1}{2}\Sigma'\,\Gamma^{(2)}\,\Sigma' \tag{20.180}$$

where in euclidean space

$$\Gamma^{(2)} = -\frac{N}{2}\left[\frac{1}{g_0} + I(q)\right] \tag{20.181}$$

with [see (9.152), (9.161), and (9.165)]

$$\begin{aligned} I(q) &= \int \frac{d^D k}{(2\pi)^D} \frac{1}{k_E^2 (k+q)_E^2} = -\left(1-\frac{D}{2}\right)\frac{D}{4} b'_\varepsilon \mu^{-\varepsilon} \left(\frac{q_E^2}{\mu^2}\right)^{-\varepsilon/2} \\ &\times \frac{\Gamma^2(1-\varepsilon/2)}{\Gamma(2-\varepsilon)} = c_\varepsilon \mu^{-\varepsilon} \left(\frac{q_E^2}{\mu^2}\right)^{\varepsilon/2}, \end{aligned} \tag{20.182}$$

where we have replaced b'_ε by

$$c_\varepsilon \equiv -\left(1-\frac{D}{2}\right)\frac{D}{4} b'_\varepsilon \approx \frac{1}{8\pi^2 \varepsilon}. \tag{20.183}$$

Thus we obtain a propagator for the collective field Σ':

$$G_{\Sigma'\Sigma'} = -\frac{2i}{N}\mu^\varepsilon \frac{1}{1/g_0\mu^{-\varepsilon} + c_\varepsilon \left(q_E^2/\mu^2\right)^{-\varepsilon/2}} \tag{20.184}$$

For $g_0 > 0$ with $g < g^*$, this is a physically acceptable quantity. For $g_0 < 0$ with $g > g^*$, however, there is a tachyon pole at

$$\frac{q_E^2}{\mu^2} = \left(\frac{-1}{g_0 \mu^{-\varepsilon} c_\varepsilon}\right)^{-2/\varepsilon} \tag{20.185}$$

as an indication that we have expanded around the wrong vacuum $\lambda_0 = 0$. We must insert the spontaneously generated mass and find that this solution must be rejected since it has a tachyon pole. The same observation was made in Subection 17.3.1 for $D = 4$, in the phase with $g_0 > 0$, which here is equivalent to $g > g^*$.

Alternatively, we can see that in the gap equation near four dimensions

$$\frac{1}{g_0 \mu^{-\varepsilon}} = \frac{1}{g} - \bar{S}_4 \frac{1}{\varepsilon}, \tag{20.186}$$

a finite renormalized coupling g can only be achieved in the limit $\varepsilon \to 0$ for negative $g_0 < 0$ in which case the ϕ^4 potential turns the wrong way around. In this case the only consistent solution for $\varepsilon \to 0$ is the free one with $g = 0$. We now realize the difference with the $N \to \infty$ Fermi case. There were two possible consistent phases, one in which a mass was spontaneously generated which was the phase which was the one with $g > g^*, g_0 < 0$ and another one for $g < g^*$ where the fermions remain massless. Here only the phase which remains massless with $\delta < g^*, g_0 > 0$ is acceptable.

The four-dimensional theory has no consistent ground state, with $\lambda = 0$, except for $g = 0$. In contrast, the three-dimensional does have one for $g < g^* \sim 8\pi^2\varepsilon$.

In the Gross-Neveu model we pointed out the existence of certain power laws in the massive phase. One concerned the physical mass as a function of $g - g^*$ or $T - T^c$ [see (20.77)], the other was a power law for $v(\Sigma) \sim \Sigma$ at the critical point

$g = g^*$, i.e., at $T = T_c$. For $T \neq T_c$, this power was still found in the UV limit $\Sigma \gg M$, while for $\Sigma \ll M$ we found the IR free point law $v(\Sigma) \sim \Sigma^2$.

We now show that the O(N)-symmetric ϕ^4 theory shows quite a similar power behavior which, however, is opposite as far as IR and UV limits are concerend. For this the mass parameter m_0^2 has to be set proportional to $T/T_c - 1$, and the critical theory will be obtained in the limit $m_0 \to 0$. In order to see this, consider the potential (20.173):

$$\frac{1}{N}v(\Phi, \lambda(\Phi_a^2)) = \frac{1}{2N}\lambda\Phi_a^2 + \frac{m_0^2}{2g_0}\lambda - \frac{1}{4g_0}\lambda^2 - \frac{b'_\varepsilon}{4}\lambda^{D/2} - \frac{m_0^4}{4g_0}, \tag{20.187}$$

where $\lambda(\Phi_a^2)$ is the function of Φ_a^2 for which $v_\lambda(\Phi, \lambda) = 0$:

$$\frac{1}{N}\Phi_a^2 = \frac{1}{g_0}\lambda - \frac{m_0^2}{g_0} + \frac{b'_\varepsilon}{2}\frac{D}{2}\lambda^{1-\varepsilon/2}. \tag{20.188}$$

Suppose we are in the normal phase $\Phi_a = 0$ and $\lambda_0 \neq 0$, and consider the critical regime with vary small m_0^2. Then from (20.167), we see λ to behave as a function of $m_0^2 \to 0$ as

$$\lambda \sim (m_0^2)^{1/(1-\varepsilon/2)}. \tag{20.189}$$

Inserting this into (20.187), we obtain for the minimal value of $v(\Phi, \lambda(\Phi_a^2))$ the power behavior

$$v_{\min} \sim (m_0^2)^{1+1/(1-\varepsilon/2)}. \tag{20.190}$$

At the critical point with $m_0 = 0$, we have

$$\frac{1}{N}\Phi_a^2 = \frac{1}{g_0}\lambda + b'_\varepsilon\frac{D}{4}\lambda^{1-\varepsilon/2}. \tag{20.191}$$

Contrary to the Gross-Neveu model there is no pure power behavior. Only if also $g_0 = 0,\ g = 0$ (free theory) or $g_0 = \infty\ \ (g = g^*)$, a pure power behavior is obtained:

$$\begin{array}{llll} \Phi_a^2 \sim \lambda, & g_0 = 0 & g = 0 & (\text{or}\ \ \lambda \to \infty), \\ \Phi_a^2 \sim \lambda^{1-\varepsilon/2}, & g_0 = \infty & g = g^* & (\text{or}\ \ \lambda \to 0). \end{array} \tag{20.192}$$

The same behavior is found at any coupling strength for $\lambda \to 0$ (ultraviolet limit) or $\lambda \to \infty$ (infrared limit), respectively. In the renormalized form of (20.192)

$$\frac{1}{N}\Phi_a^2 = \mu^\varepsilon\left\{\frac{1}{g} - b'_\varepsilon\left[1 - \frac{D}{4}\left(\frac{\lambda}{\mu^2}\right)^{-\varepsilon/2}\right]\right\}\lambda, \tag{20.193}$$

the two limits are separated by the scale parameter μ. For small λ, the potential itself behaves like

$$v(\Phi) \sim (\Phi^2)^{1+1/(1-\varepsilon/2)}, \tag{20.194}$$

as determined by the first and last term in (20.173). The small-λ behavior can be collected in the single formula valid for m_0^2

$$v(\Phi) \sim \left[m_0^2\left(\frac{\Phi^2}{m_0^2}+\frac{N}{g_0}\right)\right]^{1+1/(1-\varepsilon/2)}, \tag{20.195}$$

which follows from writing (20.188) as

$$\frac{1}{N}\Phi_a^2+\frac{m_0^2}{g_0}\sim b_\varepsilon'\frac{D}{4}\lambda^{1-\varepsilon/2}, \tag{20.196}$$

valid for small and vanishing λ and reinserting, this into (20.187).

If Φ is interpreted as magnetization M and $m_0^2 \approx (T/T_c-1)$ as the deviation of the temperature from the critical value, this corresponds to a general power law

$$v(M)\sim M^{\delta+1}f\left(\frac{T/T^c-1}{M^{1/\beta}}\right) \tag{20.197}$$

which was first observed experimentally by Widom in magnetic systems. In the present model:

$$\beta=\frac{1}{2}, \qquad \frac{\delta+1}{2}=\frac{2-\varepsilon/2}{1-\varepsilon/2}. \tag{20.198}$$

For large λ (UV-limit), there is again free field power behavior

$$\frac{1}{N}\Phi_a^2+\frac{m_0^2}{g_0}\sim\lambda \tag{20.199}$$

$$v\sim\left(\frac{\Phi_a^2}{N}+\frac{m_0^2}{g}\right)^2. \tag{20.200}$$

Note that there is great similarity with the Gross-Neveu model, as far as power behaviors are concerned. But the scaling limits are opposite. In the Gross-Neveu model, there is only one scale, the fermion mass M or the distance, of g from g^* (i.e., T from T_c). The mass M separates UV and IR limits. Once at T_c where $M=0$ there are pure powers. Away from T_c there are different powers in the UV and IR limit with $M=0$ agreeing with the UV limit. In the ϕ^4 theory, the massless theory at the point $m_0^2=0$ still has freedom in the coupling. It can be anywhere between 0 and g^*. At both ends there are pure powers. In between there are powers in the IR and UV limit. If m_0 is taken away from zero, there are more power laws in $m_0^2\sim(T/T^c-1)$ for fields and potential.

20.10 Two Phase Transitions in Chiral Gross-Neveu Model

We shall now demomonstrate that the chiral Gross-Neveu model in $2+\epsilon$ dimensions has for a small number N of fermions two phase transitions corresponding to *pair formation* and *pair condensation.*[6]

In the first transition, fermions and antifermions acquire spontaneously a mass and are bound to pairs which behave like a Bose liquid in a chirally symmetric state. In the second transition, the Bose liquid condenses into a coherent state which breaks chiral symmetry. This suggests the possibility that in particle physics, the generation of quark masses may also happen separately from the breakdown of chiral symmetry.[7]

Starting point of our discussion is Eq. (20.139) for the propagator of the massless Goldstone modes of the pair field in $D = 2+\epsilon$ dimensions:

$$G_{\Delta'_{\rm im}\Delta'_{\rm im}} = \frac{1}{N}\frac{4}{\epsilon}\left(\frac{1}{g^*} - \frac{1}{g}\right)^{-1} M^{2-\epsilon}\frac{i}{q^2} + \text{regular part at } q^2 = 0. \quad (20.201)$$

The sign of the pole term guarantees a positive norm of the corresponding particle state in the Hilbert space.

The residue of the pole term will allow us to conclude that the chiral model has two phase transitions. Consider first the case $\epsilon = 0$ where the collective field theory consists of complex field Δ with O(2)-symmetry $\Delta \to e^{i\phi}\Delta$. From the discussion of the Kosterlitz-Thouless in Section 19.2.5 that a complex field system possesses macroscopic excitations of the form of vortices and antivortices. These attract each other by a logarithmic Coulomb potential, just like a gas of electrons an positrons in two dimensions. At low temperatures, the vortices and antivortices form bound pairs. The grand-canonical ensemble of pairs exhibits quasi-long-range correlations. At some temperature T_c, the vortex pairs break up, and the correlations becomes short-range. The phase transition is of infinite order.

We have shown in Subsection 19.2.5 that this transition is most easily understood in a model field theory involving of a pure phase field $\theta(x)$, with a Lagrange density

$$\mathcal{L} = \frac{\beta}{2}[\partial\theta(x)]^2, \quad (20.202)$$

where β is the stiffness of the θ-fluctuations. The important feature of the phase field θ is that it is a cyclic field with $\theta = \theta + 2\pi$. In order to ensure that such jumps by 2π carry no energy, the gradient in the Lagrange density needs a modification which allows for the existence of vortices and antivortices.[8] After including vortices and antivortices at positions x_i, x_j, their partition function can be written as [recall (19.2.5)]

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[6] H. Kleinert and E. Babaev, Phys. Lett. B *438*, 311 (1998) (hep-th/9809112).

[7] This has been shown in the paper cited in Footnote 3.

[8] For details see H. Kleinert, *Proceedings of a NATO Advanced Study Institute on Formation and Interactions of Topological Defects* at the University of Cambridge, England (cond-mat/9503030) and the textbook H. Kleinert, *Gauge Fields in Condensed Matter*, World Scientific, 1989 (http://www.physik.fu-berlin.de/˜kleinert/kleiner_re.html#b1).

$$Z=\sum_{\rm gas}\exp\left\{4\pi^2\beta\sum_{i<j}q_iq_i\,\frac{1}{2\pi}\log(|x_i-x_j|/r_0)\right\}, \tag{20.203}$$

where r_0 characterizes the size of the vortices. For a single vortex-antivortex pair, the average square distance r^2 diverges as the stiffness falls below [recall (19.43)]

$$\beta_{\rm KT}=1/T_{\rm KT}=2/\pi\approx 0.63662. \tag{20.204}$$

The large-stiffness state with bound vortex pairs has a coherent phase field $\theta(x)$, the low-stiffness state with separated vortex pairs exhibits incoherent phase fluctuations. The same situation is found in three dimensions, only that the excitations are vortex lines. These become infinitely long and prolific in a second-order phase transition at a critical point $\beta_c\approx 0.33$.

The result (20.201) for $\epsilon=0$ can now be used to estimate a critical value of the number of field components $N=N_c$ below which the phase fluctuations of the complex field Δ' become so violent that the system has a phase transition. For this we write $\Delta'_{\rm im}=M\theta$ and find from (20.201) a propagator of the θ-field

$$G_{\theta\theta}\;\approx\;\frac{i}{N}\frac{4\pi}{q^2}+\text{regular terms}. \tag{20.205}$$

Comparing this with the propagator for the model Lagrange density (20.202)

$$G_{\theta\theta}=\frac{1}{\beta}\frac{i}{q^2} \tag{20.206}$$

we identify the stiffness $\beta=N/4\pi$. The pair version of the chiral Gross-Neveu model has therefore a vortex-antivortex pair breaking transition if N falls below the critical value $N_c=8$.

Consider now the model in $2+\epsilon$ dimensions where pairs form at $g=g^*\approx\pi\epsilon$. A comparison between the propagator (20.201) and (20.206) yields a stiffness of phase fluctuations

$$\beta=\frac{N}{4\pi}M^\epsilon\left(1-\frac{g^*}{g}\right). \tag{20.207}$$

The linear vanishing of the stiffness with the distance of the coupling constant g from the critical value g^* is in agreement with a general scaling relation, according to which the critical exponent of bending rigidity should be equal to $(D-2)\nu$.

The propagator for the real part of the pair field has, by (20.138), a correlation length

$$\xi=\left(\frac{D-1}{12M^2}\right)^{1/2}. \tag{20.208}$$

Inserting the g-dependence of M from (20.79), we see that

$$\xi=\frac{1}{M_\infty}\left(\frac{D-1}{12}\right)^{1/2}\left(1-\frac{g^*}{g}\right)^{-1/\epsilon} \tag{20.209}$$

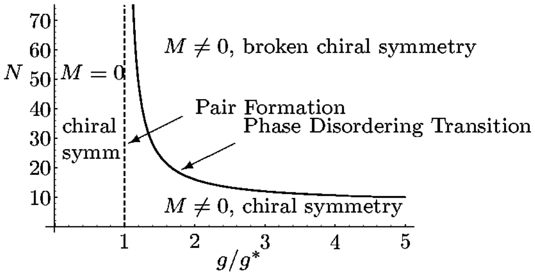

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FIGURE 20.3 The two transition lines in the $N-g$-plane of the chiral Gross-Neveu model in $2+\epsilon$ dimensions. For $\epsilon = 0$, the vertical transition line coincides with the N-axis, and the solid hyperbola degenerates into a horizontal line at $N_c = 8$. The quark masses and chiral properties are indicated.

so that the coherence length diverges for $g \longrightarrow g^*$ with a critical exponent $\nu = 1/\epsilon$.

The stiffness (20.207) implies the existence of a phase transition in the neighborhood of two and in three dimensions at roughly

$$N_c \approx 8\left(1-\frac{g^*}{g}\right)^{-1}, \quad D \approx 2, \qquad N_c \approx 4.19\left(1-\frac{g^*}{g}\right)^{-1}, \quad D = 3. \quad (20.210)$$

As N is lowered below these critical values, the phase fluctuations of the pair field Δ become incoherent and the pair condensate dissolves. The different phases are indicated in Fig. 20.3. In the chiral formulation of the same model, the intermediate phase has chiral symmetry in spite of a nonzero spontaneously generated "quark mass" $M \neq 0$. The reason why this is possible is that the "quark mass" depends only on $|\Delta_0|$, thus allowing for arbitrary phase fluctuations preserving chiral symmetry.

The sceptical reader may wonder whether the solid hyperbola in Fig. 20.3 is not simply the proper (albeit approximate) continuation of the vertical line for smaller N. There are two simple counterarguments. One is formal: For infinitesimal ϵ the first transition lies precisely at $g = g^* = \pi\epsilon$ for *all* N, so that the horizontal transition line is clearly distinguished from it. The other argument is physical. If N is lowered at some very large g, the binding energy of the pairs *increases with* $1/N$ {in two dimensions, the binding energy is $4M\sin^2[\pi/2(N-1)]$}. It is then impossible that the phase fluctuations on the horizontal branch of the transition line, which are low-energy excitations, unbind the strongly bound pairs. This will only happen in the limit $N \longrightarrow \infty$ where the binding energy becomes zero and the two transition curves merge into a single curve. This is the situation in the theory of superconductivity, where Cooper pair binding and pair condensation coincide.

In the ordinary Gross-Neveu model, the analog of the phase disordering transition is an Ising transition, in which the vacuum expectation value of σ jumps between $-\Sigma_0$ and Σ_0 in a disorderly fashion. In two dimensions, this occurs at some critical value N_c. In $2+\epsilon$ dimensions, this transition should again exist independently of the transition at which the system enters into a state of nonzero Σ_0. It will be interesting to see these two transitions in either model confirmed by Monte-Carlo simulations.

There exists a four-fimensional version of this discussion in which it is shown that, very probably, a pion condensate cannot form in the Nambu-Jona-Lasinio model, due to directional fluctuations of the pion field.[9]

20.11 Finite-Temperature Properties

It is useful to study also the behavior of the Gross-Neveu model at a finite temperature. The thermal properties of this model will closely resemble those of a superconductor. For this we confine the imaginary-time variable τ to the interval $\tau \in (0, \hbar\beta)$ with $\beta = 1/k_BT$, and take the fields to be antiperiodic under $\tau \to \tau + \hbar\beta$. Equivalently, we may think of this model as a nonlinear σ-model on an infinitely long spatial strip with antiperiodic boundary conditions, whose width along the τ-axis is β. In the limit $N \to \infty$, we can study the effects of temperature exactly. For simplicity, we consider the model only for a vanishing initial bare mass m_0. The corresponding effective potential of the Σ-field in Eq. (20.16)

$$\frac{1}{N}v(\Sigma) = -\frac{1}{N}\Gamma[\Sigma] = \frac{1}{2g_0}\Sigma^2 - \mathrm{tr}\,(1)\frac{1}{2}\int \frac{d^Dp_E}{(2\pi)^D} \log\left[p_E^2 + \Sigma^2\right] \tag{20.211}$$

is generalized to finite temperatures T by exchanging the momentum integral by a sum over Matsubara frequencies $\omega_m = \pi(2m+1)T/\hbar$, $m = 0, \pm 1, \pm 2, \dots$:

$$\int \frac{d^Dp_E}{(2\pi)^D} \to \frac{d^{D-1}p}{(2\pi)^{D-1}} \frac{1}{\hbar\beta} \sum_{\omega_m=-\infty}^{\infty}, \tag{20.212}$$

thus becoming (in natural units with $k_B = 1$ and $\hbar = 1$)

$$\frac{1}{N}v(\Sigma) = \frac{1}{2g_0}\Sigma^2 - 2^{D/2}\frac{1}{2}\int \frac{d^{D-1}p_E}{(2\pi)^{D-1}}\, T \sum_{m=-\infty}^{\infty} \log(\omega_m^2 + p_E^2 + \Sigma^2). \tag{20.213}$$

The gap equation is obtained by minimizing this action and becomes [compare (20.15)]

$$\frac{1}{g_0} = 2^{D/2}\int \frac{d^{D-1}p_E}{(2\pi)^{D-1}}\, T \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + p_E^2 + \Sigma^2}. \tag{20.214}$$

Using the well-known summation formula

$$T \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \Omega^2} = \frac{1}{2\Omega}\tanh\left(\frac{\Omega}{2T}\right), \tag{20.215}$$

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[9] See H. Kleinert and B. Van den Bossche, Phys. Lett. B **474**, 336 (2000) (hep-ph/9907274).

the gap equation becomes

$$\frac{1}{g_0} = 2^{D/2}\int\frac{d^{D-1}p_E}{(2\pi)^{D-1}}\frac{1}{2\Omega}\tanh\frac{\Omega}{2T}. \tag{20.216}$$

We shall renormalize this by adding and subtracting, on the right-hand side, the zero-temperature limit:

$$\frac{1}{g_0} = 2^{D/2}\int\frac{d^{D-1}p_E}{(2\pi)^{D-1}}\frac{1}{p_E^2+\Sigma^2}+2^{D/2}\int\frac{d^{D}p_E}{(2\pi)^{D}}\frac{1}{2\Omega}\left(\tanh\frac{\Omega}{2T}-1\right). \tag{20.217}$$

Near two dimensions, the first integral can be written as

$$2^{D/2-1}S_D\Gamma(D/2)\Gamma(1-D/2)(\Sigma^2)^{D/2-1} = b_\epsilon\frac{D}{2}\Sigma^\epsilon \approx b_\epsilon\mu^\epsilon - \frac{\mu^\epsilon}{\pi}\left(\log\frac{\Sigma}{\mu}+\frac{1}{2}\right)+\mathcal{O}(\epsilon). \tag{20.218}$$

where we have used Eqs. (20.17), (20.20). The renormalized gap equation reads then, at $\epsilon = 0$,

$$\frac{1}{g_R(\mu^2)} = \frac{1}{\pi}\log\frac{\Sigma}{\mu}+\frac{1}{2}+\frac{1}{\pi}\int_0^\infty\frac{dp}{\Omega}\left(\tanh\frac{\Omega}{2T}-1\right). \tag{20.219}$$

It is convenient to express the zero-temperature part of this equation without the arbitrary scale parameter μ, using the renormalization invariant mass

$$M = \mu\exp\left[-\frac{\pi}{g_R(\mu)}-\frac{1}{2}\right]$$

which solves the zero-temperature gap equation. Then we arrive at the finite equation

$$\frac{1}{\pi}\log\frac{\Sigma}{\Sigma_0} = \frac{1}{\pi}S_1\left(\frac{\Sigma}{2\pi T}\right), \tag{20.220}$$

with the function [compare with the bosonic version of this in Eq. (18.112)]

$$S_1\left(\frac{\Sigma}{2\pi T}\right) = \int_0^\infty\frac{dp}{\Omega}\left(\tanh\frac{\Omega}{2T}-1\right) = -2\int_0^\infty dp\,\frac{1}{\Omega}\left(e^{\Omega/T}+1\right)^{-1}. \tag{20.221}$$

This function accounts for all finite-temperature effects. It depends only on the dimensionless ratio Σ/T. We have divided this by one more factor 2π for later convenience. The dimensionless ratio $\Sigma/2\pi T$ will in the following be denoted by $\hat{\Sigma}$, i.e.,

$$\hat{\Sigma} = \frac{\Sigma}{2\pi T}. \tag{20.222}$$

The solution $\Sigma(T) \equiv M(T)$ of (20.220) is now the temperature-dependent fermion mass. For $T = 0$, the function $S_1(\hat{\Sigma})$ vanishes and $\Sigma(0) = \Sigma_0 = M$. As the temperature rises, the fermion mass $M(T)$ decrease, until it vanishes at a certain critical temperature T_c. The value of T_c is found by assuming $\Sigma(T)$ to be small, and approximating the right-hand side of (20.221) by

$$2\int_0^\infty \frac{dp}{2\pi}\left[\frac{1}{p}\tanh\left(\frac{p}{2T}\right)-\frac{1}{\sqrt{p^2+\Sigma^2}}\right]. \tag{20.223}$$

Integrating the first term by parts gives

$$\frac{1}{\pi}\left\{\log\left(\frac{p}{2T}\right)\tanh\left(\frac{p}{2T}\right)\Big|_0^\infty-\int_0^\infty dx\log x\,\cosh^{-2}x\right\}. \tag{20.224}$$

The integral is convergent and equal to $-\log(4e^\gamma/\pi)$, where $\gamma=0.577\dots$ is Euler's number. This follows at once from the formula

$$\int_0^\infty dx\,x^{\mu-1}\cosh^{-2}ax=\frac{4}{(2a)^\mu}\left(1-2^{2-\mu}\right),\Gamma(\mu)\zeta(\mu-1) \tag{20.225}$$

in the limit $\mu\to 1$, where

$$\zeta(z)\equiv\sum_{k=0}^{\infty}\frac{1}{k^z} \tag{20.226}$$

is Riemann's zeta function. Using the property $\zeta(0)=-1/2$ and $\zeta'(0)=-\frac{1}{2}\log(2\pi)\Gamma'(1)=-\gamma$. The second term in (20.223) can be integrated directly with the result $\operatorname{asinh}(p/\Sigma)=\log\left[p/\Sigma+\sqrt{p^2/\Sigma^2+1}\right]$. Hence we find for (20.223)

$$\frac{1}{\pi}\left\{\left[\log\left(\frac{p}{2T}\right)\tanh\left(\frac{p}{2T}\right)-\log\left(\frac{p}{\Sigma}+\sqrt{\frac{p^2}{\Sigma^2}+1}\right)\right]_0^\infty+\log\left(\frac{4e^\gamma}{\pi}\right)\right\}=\frac{1}{\pi}\log\left(\Sigma\frac{2e^\gamma}{\pi T}\right), \tag{20.227}$$

and (20.220) determines the critical temperature by the equation

$$\log\left(\frac{\Sigma}{\Sigma_0}\right)=\log\left(\Sigma\frac{e^\gamma}{\pi T}\right), \tag{20.228}$$

or

$$T_c=\Sigma_0\frac{e^\gamma}{\pi}=M\frac{e^\gamma}{\pi}. \tag{20.229}$$

At this temperature, the fermion mass $M(T)$ vanishes.

In order to study the full temperature behavior of $M(T)$, the right-hand side of the gap equation (20.220) has to be evaluated numerically. For this purpose, we shall derive a more useful form of the gap equation. Let us go back once more to the original form (20.214) and rewrite it for $\epsilon\sim 0$ as

$$\begin{aligned}\frac{1}{g_0}-2^{D/2}\int\frac{d^Dp}{(2\pi)^D}\frac{1}{p^2+\Sigma^2}&=\frac{1}{g_0}-b_\epsilon\mu^\epsilon+\frac{1}{2\pi}\left(\log\frac{\Sigma^2}{\mu^2}+1\right)\\&=\frac{1}{\pi}S_1(\hat\Sigma)=T\sum_{m=0}^{\infty}\frac{1}{\sqrt{\omega_m^2+\Sigma^2}}-\int_0^\infty\frac{d\omega_m}{2\pi}\frac{1}{\sqrt{\omega_m^2+\Sigma^2}}\end{aligned} \tag{20.230}$$

[compare (20.44)]. This can again be written as in (20.220):

$$\log \frac{\Sigma}{\Sigma_0} = S_1(\hat{\Sigma}), \tag{20.231}$$

where S_1 is given by the sum minus integral

$$S_1(\hat{\Sigma}) = \left(\sum_{m=0}^{\infty} - \int_{-1/2}^{\infty} dm \right) \frac{1}{\sqrt{\left(m+\frac{1}{2}\right)^2 + \Sigma_T^2}}. \tag{20.232}$$

It is useful to reorganize the sum as follows:

$$\begin{aligned} S_1(\hat{\Sigma}) &= \sum_{m=0}^{\infty} \left(\frac{1}{\sqrt{\left(m+\frac{1}{2}\right)^2 + \Sigma_T^2}} - \frac{1}{m+\frac{1}{2}} \right) \\ &+ \sum_{m=0}^{\infty} \frac{1}{m+\frac{1}{2}} - \int_{-1/2}^{\infty} dm \frac{1}{\sqrt{\left(m+\frac{1}{2}\right)^2 + \hat{\Sigma}^2}}. \end{aligned} \tag{20.233}$$

The integral up to some large $m = \bar{m}$ gives $\operatorname{asinh}(\bar{m}/\hat{\Sigma}) \rightarrow \log(2\bar{m}/\hat{\Sigma})$. The sum over $1/(m+\frac{1}{2})$ is $\gamma + \log 4 + \psi\,(\bar{m}+3/2) = \gamma + \log 4 + \psi\,(\bar{m}+1/2) + 1/(\bar{m}+1/2)$. Using the large-$z$ behavior $\psi\,(\bar{m}+1/2) \approx \log -1/2\bar{m} - 1/4\bar{m}^2$, we find for the sum the limit $\gamma + \log 4 + \log \bar{m}$, and for $S_1(\hat{\Sigma})$ the convergent sum

$$\begin{aligned} S_1(\hat{\Sigma}) &= \sum_{m=0}^{\infty} \left[\frac{1}{\sqrt{\left(m+\frac{1}{2}\right)^2 + \hat{\Sigma}^2}} - \frac{1}{m+\frac{1}{2}} \right] + \log\left(2e^{\gamma}\hat{\Sigma}\right) \\ &\equiv \tilde{S}_1(\hat{\Sigma}) + \log(2e^{\gamma}\hat{\Sigma}). \end{aligned} \tag{20.234}$$

The logarithm of $\hat{\Sigma}$ cancels a similar term on the left-hand side of the gap equation (20.220), and using the connection (20.229) between Σ_0 and the critical temperature, and substituting M for Σ_0, we obtain the gap equation in a form most suitable for a numerical evaluation:

$$\log \frac{T}{T_c} = \tilde{S}_1(\hat{\Sigma}). \tag{20.235}$$

This can be used to calculate T/T_c and $M(T) = \Sigma = 2\pi T \hat{\Sigma}$ as a function of $\hat{\Sigma}$. The resulting function $M(T)$ is plotted in Fig. 20.4.

It is quite easy to calculate the way in which $M(T)$ vanishes as T approaches the critical temperature. We simply expand

$$\begin{aligned} \tilde{S}_1(\hat{\Sigma}) &= \sum_{k=1}^{\infty} \binom{-1/2}{k} \hat{\Sigma}^{2k} \sum_{m=0}^{\infty} \frac{1}{\left(m+\frac{1}{2}\right)^{2k+1}} \\ &= -\frac{1}{2}\hat{\Sigma}^2 \sum_{m=0}^{\infty} \frac{1}{\left(m+\frac{1}{2}\right)^3} + \frac{3}{8}\hat{\Sigma}^4 \sum_{m=0}^{\infty} \frac{1}{\left(m+\frac{1}{2}\right)^5} - \dots . \end{aligned} \tag{20.236}$$

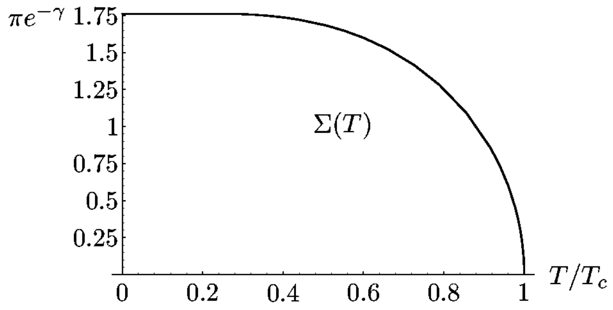

FIGURE 20.4 Solution of the temperature dependent gap equation, showing the decrease of the fermion mass $M(T)=\Sigma(T)$ with increasing temperature T/T_c.

Expanding near T_c the logarithm as $\log(T/T_c) \sim T/T_c - 1$, we find in a first approximation

$$M(T)=\Sigma \approx \pi T_c\sqrt{\frac{8}{7\zeta(3)}}\sqrt{1-\frac{T}{T_c}}. \tag{20.237}$$

In the opposite limit of low temperatures, the series (20.236) converges very slowly. It is, however, easy to find out how Σ behaves near $T=0$ by expanding in (20.221)

$$\tanh\frac{\Omega}{2T}-1=2\sum_{\tilde{m}=1}^{\infty}(-)^{\tilde{m}}e^{-\tilde{m}\Omega/T}. \tag{20.238}$$

Using the integral

$$\int_{-\infty}^{\infty} dp\,\frac{e^{-\tilde{m}\sqrt{p^2+\Sigma^2}/T}}{\sqrt{p^2+\Sigma^2}}=2K_0\left(\tilde{m}\Sigma/T\right), \tag{20.239}$$

where $K_0(z)$ is the associated Bessel function, we find the alternative expression

$$\log\frac{\Sigma}{\Sigma_0}=S_1(\hat{\Sigma})=2\sum_{\tilde{m}=1}^{0}(-)^{\tilde{m}}K_0\left(2\pi\tilde{m}\hat{\Sigma}\right). \tag{20.240}$$

For small T, $K_0\left(\tilde{m}\Sigma/T\right)$ has the asymptotic behaviour

$$K_0\left(\frac{\tilde{m}\Sigma}{T}\right)\sim\sqrt{\frac{\pi}{2\tilde{m}\Sigma/T}}e^{-\hat{\Sigma}/T}, \tag{20.241}$$

so that we can expand

$$\Sigma=\Sigma_0\left(1-\sqrt{\frac{2\pi}{\Sigma_0/T}}e^{-\Sigma/T}\right)+\mathcal{O}\left(e^{-2\Sigma/T}\right) \tag{20.242}$$

and see that Σ approaches its $T=0$ -value Σ_0 exponentially fast from below (see Fig. 20.4).

Note that the properties of the gap equation (20.220) are quite similar to those of the corresponding equation (18.110) in the nonlinear σ-model.

It is instructive to go through the same discussion once more in D dimensions. For this it is convenient to rewrite the gap equation (20.230) in accordance with the general procedure of dimensional regularization in Section 9.5 as

$$\frac{1}{g_0}-2^{D/2}\int_0^\infty d\tau\int\frac{d^Dp}{(2\pi)^D}e^{-\tau(p^2+\Sigma^2)}=\frac{\Sigma^{D-2}}{\pi}2^{1-D/2}\pi^{(1-D)/2}\Gamma(3/2-D/2)S_1(\hat{\Sigma}). \tag{20.243}$$

The left-hand side corresponds to the zero-temperature gap equation and is integrated directly to

$$\frac{1}{g_0}-b_\epsilon\frac{D}{2}\Sigma^\epsilon=\frac{\mu^\epsilon}{g(\mu)}-b_\epsilon\left(\frac{D}{2}\Sigma^\epsilon-\mu^\epsilon\right), \tag{20.244}$$

while

$$\begin{aligned}S_1(\hat{\Sigma}) &= \pi\Sigma^{2-D}2^{D-1}\pi^{(D-1)/2}\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\right]^{-1} \\ &\times \int_0^\infty d\tau\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\left(T\sum_{m=-\infty}^{\infty}-\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\exp\left[-\tau\left(\omega_m^2+p^2+\Sigma^2\right)\right].\end{aligned} \tag{20.245}$$

The mometum integrations can now be done, with the result

$$\frac{1}{g_0}-2^{D/2}\frac{1}{2^D}\pi^{-D/2}\int_0^\infty\frac{d\tau}{\tau^{D/2}}e^{-\tau\Sigma^2}=\Sigma^{D-2}2^{1-D/2}\pi^{-1/2-\frac{D}{2}}\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)S_1(\hat{\Sigma}), \tag{20.246}$$

where

$$S_1(\hat{\Sigma})=2\pi\Sigma^{2-D}\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\right]^{-1}\int_0^\infty\frac{d\tau}{\tau^{D/2-1}}\left(T\sum_{m=0}^{\infty}-\int_0^\infty\frac{d\omega_m}{2\pi}\right)e^{-\tau(\omega_m^2+\Sigma^2)}. \tag{20.247}$$

By performing the τ-integral on the right-hand side, we find

$$\begin{aligned}S_1(\hat{\Sigma}) &= 2\pi\Sigma^{2-D}\left(T\sum_{m=0}^{\infty}-\int_0^\infty\frac{d\omega_m}{2\pi}\right)(\omega_m^2+\Sigma^2)^{(D-3)/2} \\ &= \hat{\Sigma}^{2-D}\left(\sum_{m=0}^{\infty}-\int_{-1/2}^{\infty}dm\right)\left[\left(m+\frac{1}{2}\right)^2+\hat{\Sigma}^2\right]^{(D-3)/2}.\end{aligned} \tag{20.248}$$

Let us expand the sum over m formally in a power series of $\hat{\Sigma}$. Its its contributions to $S_1(\hat{\Sigma})$ is

$$S_1(\hat{\Sigma})\Big|_{\rm sum\ part}=\hat{\Sigma}^{2-D}\sum_{k=0}^{\infty}\left(\begin{array}{c}(D-3)/2\\ k\end{array}\right)\hat{\Sigma}^{2k}\zeta\left(2k+3-D,1/2\right), \tag{20.249}$$

where

$$\zeta(z,a)\equiv\sum_{k=0}^{\infty}\frac{1}{(k+n)^z} \tag{20.250}$$

is Riemann's zeta function with $\zeta(z,1)=\zeta(z)$ of Eq. (20.226). The integral over ω_m in (20.248) subtracts from this the $T=0$ -limit of (20.249):

$$2^{D/2-1}\pi^{(D-1)/2}\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\right]^{-1}b_\epsilon\frac{D}{2}\pi=\frac{\sqrt{\pi}}{2}\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\right]^{-1}\Gamma\left(1-\frac{D}{2}\right).\quad(20.251)$$

For D near an even dimension $\bar{D}$, say $D=\bar{D}+\epsilon$, the kth term with $k=\bar{D}/2-1$ has an $1/\epsilon$-singularity coming from the zeta function

$$\zeta\left(1+\bar{D}-D,1/2\right)\sim\frac{1}{\epsilon}\left[1+\epsilon\psi\left(1/2\right)\right].\quad(20.252)$$

This is canceled by a singularity of opposite sign in b_ϵ. We now expand up to first order in ϵ:

$$\begin{aligned}&\hat{\Sigma}^{2-D}\binom{(D-3)/2}{k}_{k=\bar{D}/2}\hat{\Sigma}^{\bar{D}-2}\zeta\left(1-\epsilon,1/2\right)=\frac{\Gamma((D-1)/2)}{\Gamma(\bar{D}/2)\Gamma(1/2+\epsilon/2)}\hat{\Sigma}^{-\epsilon}\zeta\left(1-\epsilon,1/2\right)\\&\approx\frac{1}{\Gamma\left(3/2-D/2\right)\Gamma(\bar{D}/2)\Gamma(1/2)}\frac{\pi}{\cos\pi\left(\bar{D}/2-1\right)}\frac{-1}{\epsilon}\left\{1+\frac{\epsilon}{2}\left(-2\log\hat{\Sigma}+\psi(1/2)\right)\right\}\\&\approx-\frac{(-1)^{\bar{D}/2}}{\Gamma\left(3/2-D/2\right)\Gamma(\bar{D}/2)}\frac{\sqrt{\pi}}{\epsilon}\left\{1+\frac{\epsilon}{2}\left[-2\log\hat{\Sigma}+\psi(1/2)+\psi\left(3/2-\bar{D}/2\right)\right]\right\}\end{aligned}$$

Similarly we expand the $T=0$ -term (20.251):

$$\begin{aligned}&\frac{\sqrt{\pi}}{2}\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\right]^{-1}\Gamma\left(1-\frac{D}{2}\right)\\&\qquad=\frac{(-)^{\bar{D}/2}}{\Gamma(\bar{D}/2)\Gamma(3/2-\bar{D}/2)}\frac{\sqrt{\pi}}{\epsilon}\left\{1-\frac{\epsilon}{2}\left[\psi(\bar{D}/2)-\psi\left(3/2-\bar{D}/2\right)\right]\right\}.\quad(20.253)\end{aligned}$$

Subtracting the two terms from each other yields

$$\begin{aligned}&-\frac{(-)^{\bar{D}/2}}{\Gamma(\bar{D}/2)\Gamma(3/2-\bar{D}/2)}\frac{\sqrt{\pi}}{2}\left[2\log\hat{\Sigma}-\psi\left(1/2\right)-\psi\left(\bar{D}/2\right)\right]\\&\qquad=-\frac{(-)^{\bar{D}/2}}{\Gamma(\bar{D}/2)\Gamma(3/2-D/2)}\frac{\sqrt{\pi}}{2}\left[2\log(2e^{\gamma}\hat{\Sigma})-\psi\left(\bar{D}/2\right)-\gamma\right].\quad(20.254)\end{aligned}$$

On the right-hand side we may replace the Digamma function $\psi(\bar{D}/2)$ for $\bar{D}=2$ by $\psi(\bar{D}/2)=-\gamma$, and for $\bar{D}>2$, $\psi(\bar{D}/2)=-\gamma+2/\bar{D}+\ldots+2/(\bar{D}-2)$. Going now to the limit $\epsilon\rightarrow 0$, we obtain for even $D=\bar{D}$:

$$\begin{aligned}S_1(\hat{\Sigma})&=-\frac{(-)^{D/2}}{\Gamma(D/2)\Gamma(3/2-D/2)}\frac{\sqrt{\pi}}{2}\left[2\log(2e^{\gamma}\hat{\Sigma})-\psi(D/2)-\gamma\right]\\&+\sum_{k=0,k\neq D/2-1}^{\infty}\binom{(D-3)/2}{k}\hat{\Sigma}^{2k+2-D}\zeta\left(2k+3-D,1/2\right).\quad(20.255)\end{aligned}$$

By taking the negative powers of $\hat{\Sigma}^2$ out of the sum, we split

$$\begin{aligned} S_1(\hat{\Sigma}) &= -\frac{(-)^{D/2}}{\Gamma(D/2)\Gamma(9/2-D/2)}\frac{\sqrt{\pi}}{2}\left[2\log\left(2e^{\gamma}\hat{\Sigma}\right)-\psi(D/2)-\gamma\right] \\ &+\sum_{k}^{D/2-2}\binom{(D-3)/2}{k}\hat{\Sigma}^{2k+2-D}\zeta\left(2k+3-D,1/2\right)+\tilde{S}_1(\hat{\Sigma}), \end{aligned} \tag{20.256}$$

where

$$\tilde{S}_1(\hat{\Sigma}) \equiv \sum_{k=D/2}^{\infty}\binom{(D-3)/2}{k}\hat{\Sigma}^{2k+2-D}\zeta\left(2k+3-D,1/2\right). \tag{20.257}$$

The sum $\tilde{S}_1(\hat{\Sigma})$ can also be calculated from the sum part in (20.248) by performing $D/2$ subtractions:

$$\begin{aligned} \tilde{S}_1(\hat{\Sigma}) = \hat{\Sigma}^{2-D}\sum_{m=0}^{\infty}&\left\{\left[\left(m+\frac{1}{2}\right)^2+\hat{\Sigma}^2\right]^{(D-3)/2}\right. \\ &\left.-\left(m+\frac{1}{2}\right)^{D-3}-\frac{D-3}{2}\hat{\Sigma}^2\left(m+\frac{1}{2}\right)^{D-5}+\dots\right\}. \end{aligned} \tag{20.258}$$

This sum is convergent and starts out with $\tilde{S}_1(0)=0$. It is the generalization of $\tilde{S}_1(\hat{\Sigma})$ in Eq. (20.234) to arbitrary even D.

Let us also generalize the other expression for $S_1(\hat{\Sigma})$ in Eqs. (20.221) and (20.240) to arbitrary D, such that it gives the finite-temperature correction to the gap equation

$$\begin{aligned} \Sigma^{-1}i\Delta_T\mathrm{tr}\frac{1}{i\partial\!\!\!/-\Sigma}(0) &= \left[2^{D/2}\int\frac{d^{D-1}p_E}{(2\pi)^{D-1}}\,T\sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+p_E^2+\Sigma^2}\right]-\Big[\dots\Big]_{T\to 0} \\ &= \frac{\Sigma^{D-2}}{\pi}2^{1-D/2}\pi^{(1-D)/2}\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)S_1(\hat{\Sigma}), \end{aligned} \tag{20.259}$$

where the notation

$$\Delta_T X(T)\equiv X(T)-X(0) \tag{20.260}$$

denotes the finite-temperature correction to any quantity $X(T)$. By comparison with (20.245), we can identify

$$\begin{aligned} S_1(\hat{\Sigma}) &= 2^{D-2}\pi^{(D+1)/2}\Sigma^{2-D}\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\right]^{-1}\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\frac{1}{\Omega}\left(\tanh\frac{\Omega}{2T}-1\right) \\ &= \pi\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\Gamma\left(\frac{D}{2}-\frac{1}{2}\right)\right]^{-1}\Sigma^{2-D}\int_0^{\infty}dp\,p^{D-2}\frac{1}{\Omega}\left(\tanh\frac{\Omega}{2T}-1\right). \end{aligned} \tag{20.261}$$

Writing $\tanh(\Omega/2T)-1$ as $-2(1+e^{\Omega/T})^{-1}$, and expanding this in powers of $e^{-\Omega/T}$, we have the alternaitve expression

$$S_1(\hat\Sigma) \;=\; 2\pi\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\Gamma\left(\frac{D}{2}-\frac{1}{2}\right)\right]^{-1}\Sigma^{2-D}\sum_{\tilde m=1}^{\infty}(-)^{\tilde m}\int_0^\infty dp\,p^{D-2}\Omega^{-1}e^{-\tilde m\Omega/T}. \tag{20.262}$$

Using the integral representation for the modified Bessel function

$$K_\nu(z)=\left(\frac{z}{2}\right)^{\nu}\frac{\Gamma(1/2)}{\Gamma(\nu+1/2)}\int_0^\infty ds s^{2\nu}(s^2+1)^{-1/2}e^{-z\sqrt{s^2+1}}, \tag{20.263}$$

we arrive at the expansion

$$S_1(\hat\Sigma) \;=\; \pi\left[\Gamma\left(\frac{3}{2}-\frac{D}{2}\right)\Gamma\left(\frac{1}{2}\right)\right]^{-1}2^{D/2}\sum_{\tilde m=1}^{\infty}(-)^{\tilde m}\left(2\pi\tilde m\hat\Sigma\right)^{1-D/2}K_{D/2-1}(2\pi\tilde m\hat\Sigma), \tag{20.264}$$

which for $D=2$ reduces properly to (20.240).

Let us also calculate the finite-temperature correction to the free energy for all dimensions D. By integrating the gap equation (20.243) with (20.244) and (20.245) in $\Sigma^2/2$, we obtain

$$\frac{1}{N}v(\Sigma)=\frac{\Sigma^2}{2g}+i\mathrm{Tr}\,\log(i\partial\!\!\!/-\Sigma)+i\Delta_T\log(i\partial\!\!\!/-\Sigma), \tag{20.265}$$

with

$$\begin{aligned} i\Delta_T\mathrm{Tr}\,\log(i\partial\!\!\!/-\Sigma) \;&=\; -2^{D/2}\int\frac{d^{D-1}p_E}{(2\pi)^{D-1}}\frac{1}{2}\left(T\sum_{m=-\infty}^{\infty}-\int_{-\infty}^{\infty}\frac{d\omega_m}{2\pi}\right)\log\left(\omega_m^2-\Omega^2\right)\\ &=\; -2^{D/2}T\int\frac{d^{D-1}p_E}{(2\pi)^{D-1}}\log\left(1+e^{-\Omega/T}\right), \end{aligned} \tag{20.266}$$

We now introduce a function $S_0(\hat\Sigma)$, so that

$$i\Delta_T\mathrm{Tr}\,\log(i\partial\!\!\!/-\Sigma)\equiv\frac{1}{N}\Delta_Tv(\Sigma)=-\frac{\Sigma^D}{\pi}2^{-D/2}\pi^{1/2-D/2}\Gamma\left(\frac{1}{2}-\frac{D}{2}\right)S_0(\hat\Sigma), \tag{20.267}$$

and find for $S_0(\hat\Sigma)$ the following expressions

$$S_0(\hat\Sigma)=4\pi\Sigma^{-D}\left[\Gamma\left(\frac{1}{2}-\frac{D}{2}\right)\Gamma\left(\frac{D}{2}-\frac{1}{2}\right)\right]^{-1}T\int_0^\infty dp\,p^{D-2}\log\left(1+e^{-\Omega/T}\right), \tag{20.268}$$

or, alternatively,

$$S^0(\hat\Sigma) \;=\; \hat\Sigma^{-D}\left(\sum_{m=0}^{\infty}-\int_{-1/2}^{\infty}dm\right)\left[\left(m+\frac{1}{2}\right)^2+\hat\Sigma^2\right]^{(D-1)/2}. \tag{20.269}$$

The new function e $S_0(\hat{\Sigma})$ is related to $S_1(\hat{\Sigma})$ by an integration

$$S_0(\hat{\Sigma}) = \frac{D-1}{2}\hat{\Sigma}^{-D}\int_0^{\hat{\Sigma}^2} d\Sigma_T^2 \left[\Sigma_T^{D-2} S_1(\hat{\Sigma})\right], \tag{20.270}$$

we can integrate (20.255)-(20.258), and see that the latter expression is separated into a convergent sum

$$\begin{aligned} \tilde{S}_0(\hat{\Sigma}) \;=\; & \hat{\Sigma}^{-D}\sum_{m=0}^{\infty}\left\{\left[\left(m+\frac{1}{2}\right)^2+\Sigma_T^2\right]^{(D-1)/2}\right. \\ & \left. -\left(m+\frac{1}{2}\right)^{(D-1)/2} - \frac{D-1}{2}\hat{\Sigma}^2\left(m+\frac{1}{2}\right)^{D-3}+\dots\right\}, \end{aligned} \tag{20.271}$$

with $D/2+1$ subtractions, an additional logarithmic term

$$\frac{(-)^{D/2}}{\Gamma(D/2)\Gamma(1/2-D/2)}\frac{\sqrt{\pi}}{2}\left[2\log(2^{\gamma}\hat{\Sigma})-\psi\left(D/2+1/2\right)-\gamma\right], \tag{20.272}$$

and a sum over negative powers of $\hat{\Sigma}$ from the integral over the second term in (20.256).

Alternatively we find from an integral (20.270) over the expansion (20.264):

$$S_0(\hat{\Sigma}) = 2\pi\, 2^{D/2}\left[\Gamma\left(\frac{1}{2}-\frac{D}{2}\right)\Gamma\left(\frac{1}{2}\right)\right]^{-1}\sum_{\tilde{m}=1}^{\infty}(-)^{\tilde{m}}\left(2\pi\tilde{m}\hat{\Sigma}\right)^{-D/2}K_{D/2}(2\pi\tilde{m}\hat{\Sigma}). \tag{20.273}$$

According to Eq. (20.270), this has to satisfy

$$\frac{d\hat{\Sigma}^D S_0}{d\hat{\Sigma}^2} = -\frac{1-D}{2}\hat{\Sigma}^{D-2}S_1, \tag{20.274}$$

and a comparison with (20.264) shows that it does, since

$$\left[z^{D/2}K_{D/2}(z)\right]' = -z^{D/2}K_{D/2-1}(z). \tag{20.275}$$

In the high-temperature limit, we use the small-z behavior

$$K_{D/2}(z) \approx \frac{1}{2}\Gamma\left(\frac{D}{2}\right)\left(\frac{z}{2}\right)^{-D/2}, \tag{20.276}$$

to find

$$S_0(\hat{\Sigma}) \approx \pi^{1-D}\hat{\Sigma}^{-D}\frac{\Gamma(D/2)}{\Gamma(1/2-D/2)}\Gamma\left(\frac{1}{2}\right)\sum_{\tilde{m}=1}^{\infty}(-1)^{\tilde{m}}(\tilde{m})^{-D}. \tag{20.277}$$

The sum can be expressed in terms of Riemann's zeta function (20.226) as

$$\sum_{\tilde{m}=1}^{\infty}(-1)^{\tilde{m}}(\tilde{m})^{-D} = -\left(1-2^{1-D}\right)\zeta(D). \tag{20.278}$$

For $D=2$, we thus obtain

$$S_0(\hat{\Sigma}) \quad \to \quad \pi \frac{T^2}{\Sigma^2}\zeta(2). \tag{20.279}$$

Recalling (20.267), this yields the low-temperature behavior of the effective potential in two dimensions

$$\frac{1}{N}\Delta_T v(\Sigma) \quad \to \quad \frac{1}{\pi}T^2\zeta(2) = \frac{T^2\pi}{6}. \tag{20.280}$$

This is the well-known free energy of a hot (or massless) Fermi Gas in two dimensions. It could have been obtained directly by dimensional regularization from the $\Sigma=0$ -expression

$$\begin{aligned} \frac{1}{N}\Delta_T v(\Sigma) &= -\int \frac{dp}{2\pi}\left(T\sum_{m=-\infty}^{\infty} - \int\frac{d\omega_m}{2\pi}\right)\log(\omega_m^2+p^2) \\ &= -T\sum_{m=-\infty}^{\infty}\sqrt{\omega_m^2} = -4\pi T^2\zeta\left(-1,1/2\right) = -T^2\frac{\pi}{6}, \end{aligned} \tag{20.281}$$

the last equation following from $\zeta\left(-1,1/2\right) = (2^{-1}-1)\zeta(-1) = 1/24$.

In $D=4$ dimensions, the result is

$$\begin{aligned} S_0(\hat{\Sigma}) &= \frac{1}{\pi^3}\hat{\Sigma}^{-4}\left[\Gamma\left(-3/2\right)\sqrt{\pi}\right]^{-1}\sum_{\tilde{m}=1}^{\infty}(-)^{\tilde{m}}\tilde{m}^{-4} \\ &= \Sigma^{-4}2^4\pi T^4\left[\Gamma\left(-3/2\right)\sqrt{\pi}\right]^{-1}\frac{7}{8}\zeta(4), \end{aligned} \tag{20.282}$$

and for the potential

$$\frac{1}{N}\Delta_T v(\Sigma) \quad \to \quad -4T^4\frac{7}{8}\frac{\pi^2}{g^D}. \tag{20.283}$$

The latter which follows directly from

$$\begin{aligned} \frac{1}{N}\Delta_T v(\Sigma) &= -2\int\frac{d^3p}{(2\pi)^3}\left(T\sum_{m=-\infty}^{\infty} - \int\frac{d\omega_m}{2\pi}\right)\log\left(\omega_m^2+p^2\right) \\ &= 2\int_0^\infty\frac{d\tau}{\tau}\int\frac{d^3p}{(2\pi)^3}T\sum_{m=-\infty}^{\infty}e^{-\tau(\omega_m^2+p^2)} \\ &= (4\pi^{3/2})^{-1}\Gamma\left(-\tfrac{3}{2}\right)T\sum_{m=-\infty}^{\infty}(\omega_m^2)^{3/2} = T^4 4\pi^{3/2}\Gamma\left(-\tfrac{3}{2}\right)\zeta\left(-3,\tfrac{1}{2}\right). \end{aligned} \tag{20.284}$$

It is the fermion equivalent to the *Stephan-Boltzmann law* for the free energy density f of hot (or massless) fermions. Compare the discussion for the bosonic model in the paragraph below Eq. (18.169), wher we show that for a pure power behavior of T^n of f, the entropy density $s=-\partial f/\partial T$ is related to f by a factor $-4/T$, whereas the internal energy density $u \equiv E/V = f + TS$ and for the specific heat at constant volume $c_V = \partial u/\partial T|_V$, carry the relative factors $1-n$ and $(1-n)n/T$, respectively.

Thus, Eq. (20.284) yields for these three thermodynamic quantities

$$f = -\frac{1}{3}u = -\frac{T}{4}s = -\frac{T}{12}c_V = -4\,\frac{2}{3}\frac{\pi^2}{60}\,\frac{7}{8}T^4. \tag{20.285}$$

In proper physical units

$$f = -\frac{1}{3}u = -\frac{T}{4}s = -\frac{T}{12}c_V = -4\,\frac{2}{3}\frac{\sigma}{c}\,\frac{7}{8}T^4, \tag{20.286}$$

where σ is the Stephan-Boltzmann constant (18.172). The prefactor 4 accounts for the two polarization degree of freedom of both particles and antiparticles, while the factor 7/8 is typical for fermions.

Recall that the black-body radiation of photons has a free energy

$$f = -\frac{1}{3}u = -\frac{T}{4}s = -\frac{T}{12}c_V = -2\,\frac{\pi^2}{90}\,T^4 = -2\,\frac{2}{3}\frac{\sigma}{c}\,T^4, \tag{20.287}$$

where the prefactor 2 on the right-hand side accounts now for the two polarization degrees of photons. In contrast to the fermion case, particles and antiparticles coincide.

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21

The Renormalization Group

In the previous chapter we have discussed some solvable models which illustrate an important aspect of the renormalization procedure: When defining renormalized quantities in a massless theory, we cannot avoid to introduce some mass parameter μ. The value of this mass parameter is a matter of choice. If the Lagrangian density contains a mass m, the role of μ can be played by m itself. But this is not always the most convenient choice. Often we want to study the limit $m \to 0$ of a theory. Then it is preferable to renormalize also a massive theory with the help of an auxiliary mass μ. As long as $m \neq 0$, this amounts to an overparametrization of the theory. This is a useful technical trick to derive the characteristic behavior of experimental observables for an important set of physical phenomena. These are the *critical phenomena* which occur as a function of temperature T in many-body systems as the T tends towards a so-called critical temperature T_c, where the system undergoes a *second-order phase transition*. At T_c, fluctuations acquire an infinitely long range corresponding to the mass m in the fields going to zero. The mass parameter vanishes near T_c like

$$m^2 = {\mu_0}^2 \left(\frac{T}{T_c} - 1 \right). \tag{21.1}$$

Suppose that we want to study the temperature behavior of a field theory in the neighborhood of $m^2 = 0$, and that we have chosen the mass m itself as the mass scale μ of renormalization. Then we are able to calculate renormalized Green functions as long as $m^2 \neq 0$. At the limiting point $m^2 = 0$, we have to change the renormalization procedure and introduce some non-zero mass scale μ. Obviously, such a procedure is not well adapted to study the limit $m \to 0$. A unified renormalization of massive and the massless case with a single arbitrary mass scale μ is preferable.

Certainly, all physical quantities must be independent of the mass parameter μ when expressed in terms of the bare quantities. Only the renormalized quantities depend on μ.

21.1 Example for Redundancy in Parametrization of Renormalized Theory

As an example, recall the situation in the O(N)-symmetric self-interacting four-fermion theory. In the limit $N \to \infty$, the effective potential reads at zero input fermion mass [recall b_ϵ from Eq. (20.20)]:

$$\frac{1}{N}v(\Sigma) = \frac{1}{2}\left(\frac{\Sigma^2}{g_0} - b_\epsilon \Sigma^{2+\epsilon}\right) = \frac{\mu^\epsilon}{2}\left[\frac{\Sigma^2}{g_0\mu^\epsilon} - b_\epsilon \left(\frac{\Sigma}{\mu}\right)^{2+\epsilon}\mu^2\right] \tag{21.2}$$

This expression is trivially independent of the mass parameter μ. The necessity for introducing the mass parameter μ arises only if we want to go to the limit of two dimensions with $\epsilon \to 0$. Then we want to define the theory with the help of a finite renormalized coupling constant, and this cannot be done without μ. The renormalized coupling constant will necessarily depend on μ, as the bare coupling constant g_0 is always held fixed. The μ-dependence is given by

$$\frac{1}{g(\mu,\varepsilon)} = \frac{1}{g_0\mu^\epsilon} - b_\epsilon. \tag{21.3}$$

To emphasize the μ-dependence at fixed g_0, as well as the dependence on ϵ, we have added these arguments to the renormalized coupling g.

In a more general renormalizable theory, all renormalized quantities are functions of μ and ϵ. Let us also make the dependence on the bare quantities explicit by writing

$$m = m(m_0, g_0, \mu.\epsilon) \tag{21.4}$$
$$g = g(m_0, g_0, \mu, \epsilon). \tag{21.5}$$

The fields are renormalized by a factor

$$\phi = \phi_0 Z_\phi^{-\frac{1}{2}}(m_0, g_0, \mu, \epsilon). \tag{21.6}$$

If we vary the mass parameter μ at fixed bare quantities, the Green functions remain the same. The renormalized quantities m, g change with μ. This implies that they are not directly experimentally observable. Experimental quantities such as particle masses and scattering amplitudes cannot depend on the dummy mass parameter μ. At $\epsilon \neq 0$, these depend only on the initial *bare* quantities. The main observable of the O(N)-symmetric four-fermion theory with zero initial mass is the fermion mass M_f arising from a spontaneous symmetry breakdown. It is given by the value of Σ' at the minimum of the potential v.

$$M_f = \left(\frac{2/D}{g_0 b_\epsilon}\right)^{1/\epsilon}. \tag{21.7}$$

In the limit $\epsilon \to 0$, the finite physical mass M_f must always be reproduced by the constant theory. Since b_ε diverges the bare coupling has to become infinitesimally small.

The mass scale μ is needed to describe the situation in the limit $\epsilon \to 0$ in terms of finite quantities. To do this, we express (21.7) in terms of the renormalized coupling g which is defined by

$$\frac{1}{g(\mu,\varepsilon)} \equiv \frac{1}{g_0\mu^{\varepsilon}} - b_{\varepsilon}, \tag{21.8}$$

as follows [using (21.3)]:

$$\frac{M_f}{\mu} = \left(\frac{2/D}{g_0\mu^{\epsilon}b_{\epsilon}}\right)^{1/\epsilon} = \left[\frac{2}{D}\left(1+\frac{1}{b_{\epsilon}g(\mu,\epsilon)}\right)\right]^{1/\epsilon}. \tag{21.9}$$

Here we can easily take the limit $\epsilon \to 0$, in which the right-hand side becomes:

$$\begin{aligned}\frac{M_f}{\mu} &= \exp\left\{\frac{1}{\epsilon}\log\left[\frac{2}{D}\left(1+\frac{1}{b_{\epsilon}g(\mu,\epsilon)}\right)\right]\right\}\\ &= \exp\left\{\frac{1}{\epsilon}\log\left[\left(1-\frac{\epsilon}{2}\right)\left(1+\frac{1}{b_{\epsilon}g(\mu,\epsilon)}\right)\right]\right\}\\ &\approx \exp\left\{\frac{1}{\epsilon}\left(-\frac{\epsilon}{2}+\frac{1}{b_{\epsilon}g(\mu,\epsilon)}-\frac{\epsilon}{b_{\epsilon}g(\mu,\epsilon)}\right)\right\}\\ &\xrightarrow{\epsilon\to 0} \exp\left\{-\left(\frac{1}{2}+\frac{\pi}{g(\mu)}\right)\right\}\end{aligned} \tag{21.10}$$

where

$$g(\mu) \equiv g(\mu, 0). \tag{21.11}$$

This equation shows very clearly how the renormalization process leads to an over-parametrisation of, the same theory by the parameter μ. The physical mass M_f is fixed, and the equation specifies in which way the renormalized coupling $g(\mu)$ depends on μ to guarantee a certain mass M_f. See Fig. 21.1 for an illustration. This relation between μ and $g(\mu)$ is typical for a large variety of theories, as we shall see in the sequel.

In general, the μ-dependence of the renormalized observables is governed by a partial differential equation called the *Callan-Symanzik equation*. This equation allows us to find curves in the space of renormalized coupling and mass parameters g, m along which a field theory has identical observables. These curves are called *renormalization group trajectories*, and the movement along them if μ is changed will be called *renormalization flow*.

Since the theory is renormalizable, the relations between observable quantities must all be finite. The model potential (21.2) illustrates this fact. Inverting relation (21.7), we express the bare coupling constant g_0 in terms of the fermion mass M_f. After inserting the result into (21.2), we obtain

$$\frac{1}{N}v(\Sigma) = \frac{{M_f}^{\epsilon}}{2}\Sigma^2\left[\frac{D}{2} - b_{\epsilon}\left(\frac{\Sigma}{M_f}\right)^{\epsilon}\right]. \tag{21.12}$$

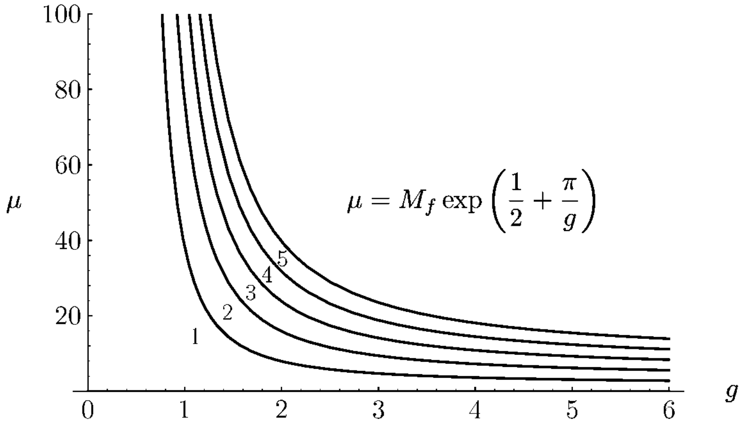

FIGURE 21.1 Curves in the (μ, g)-plane corresponding to the same physical fermion mass $M_f = 1, \ldots, 5$, and thus to identical physical observables. These curves are the renormalization group trajectories of the O(N)-symmetric four-fermion model in the limit $N \to \infty$.

This is a finite relation for all values of ϵ, in particular for $\epsilon \longrightarrow 0$ where it has the limit

$$\frac{1}{N} v(\Sigma) = \frac{\Sigma^2}{2\pi}\left[\log\left(\frac{\Sigma}{M_f}\right) - \frac{1}{2}\right]. \tag{21.13}$$

Note that by expressing $v(\Sigma)$ in terms of the physical observable M_f rather than the finite quantity $g(\mu)$, we have arrived at an expression which is finite *and* independent of μ. This $v(\Sigma)$ will be called a *renormalization-group-invariant* version of the effective potential.

We shall see that an understanding of the renormalization group will permit us to find an economic way of expressing all renormalized quantitties in such a μ-independent way. Mathematically speaking, the determination of physical oservables which do not depend on the renormalization scheme will amount to a search for invariants under the renormalization group.

To develop the theory we shall focus our attention again on the ϕ^4-theory in $D = 4 - \epsilon$ dimensions, renormalized via an ϵ-expansion.

21.2 Renormalization Scheme

In Chapter 9 we have seen how to obtain, for the ϕ^4-theory in four spacetime dimensions, all finite vertex functions $\Gamma^{(n)}(p, g, m, \mu)$ order by order in perturbation theory. Besides the physical parameters g and m, it was convenient to carry along an auxiliary mass parameter μ. The finiteness of the Feynman graphs was achieved by adding to the renormalized Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 - \frac{g\mu^\epsilon}{4!}\phi^4 \tag{21.14}$$

a corresponding set of counterterms, divergent for $\epsilon \to 0$,

$$\mathcal{L}_c = \frac{1}{2}c^{\phi}(\partial\phi)^2 - \frac{m^2}{2}c^m\phi^2 - \frac{g\mu^{\epsilon}}{4!}c^g\phi^4. \tag{21.15}$$

We have replaced the original renormalized coupling constant g by $g\mu^{\epsilon}$. As we have seen before in Chapter 9, this has the advantage of making all counterterms functions of the new dimensionless renormalized coupling constant g only [call (9.249)]. The counterterms were calculated at every order in perturbation theory from the primitively divergent diagrams (divergent means divergent in the limit $\epsilon \to 0$). Renormalizability of the theory implies that no other divergent counterterms are necessary than those which can be written in the same form as the original Lagrangian as in Eq. (21.15). Then all divergencies can be absorbed in a multiplicative redefinition of field, mass, and coupling constant. The total Lagrangian $\mathcal{L} + \mathcal{L}_c$ is

$$\mathcal{L}_0 = \mathcal{L} + \mathcal{L}_c = \frac{1}{2}(\partial\phi_0)^2 - \frac{{m_0}^2}{2}{\phi_0}^2 - \frac{g_0}{4!}{\phi_0}^4, \tag{21.16}$$

and this may be identified with the initial bare Lagrangian, in which the bare field, mass, and coupling constant are related to the finite renormalized ones by

$$\begin{aligned} \phi_0 &\equiv {Z_\phi}^{1/2}\phi, \\ {m_0}^2 Z_\phi &\equiv m^2 \bar{Z}_{m^2}, \\ g_0 {Z_\phi}^2 &\equiv g\mu^{\epsilon}\bar{Z}_g, \end{aligned} \tag{21.17}$$

with the renormalization constants

$$\begin{aligned} Z_\phi &\equiv 1 + c^{\phi}(g,\epsilon), \\ \bar{Z}_{m^2} &\equiv 1 + c^{m}(g,\epsilon), \\ \bar{Z}_g &\equiv 1 + c^{g}(g,\epsilon). \end{aligned} \tag{21.18}$$

The bare Green functions when calculated in $4 - \epsilon$ dimensions

$$G_0{}^{(n)}(x_1,\dots,x_n;g_0,m_0\epsilon) = \langle 0|T\phi_0(x_1)\dots\phi_0(x_n)|0\rangle, \tag{21.19}$$

are finite objects as long as $\epsilon \neq 0$. When multiplied by the renormalization constants ${Z_\phi}^{n/2}$, they turn into the renormalized Green functions which remain finite in the limit $\epsilon \to 0$:

$$G^{(n)}(x_1,\dots,x_n;g,m,\mu) \equiv {Z_\phi}^{n/2}(g,\epsilon)G_0{}^{(n)}(x_1,\dots,x_n;g_0,m_0,\epsilon). \tag{21.20}$$

Correspondingly, the bare vertex functions

$$\begin{aligned} \Gamma_0^{(n)}(x_1,\dots,x_n;g_0,m_0,\mu) \equiv & -i\int dx_1'\cdots dx_n' \\ & \times G_0{}^{-1}(x_1,x_1';g_0,m_0,\epsilon)\cdots G_0{}^{-1}(x_n,x_n';g_0,m_0,\epsilon)\,G_0{}^{(n)}(x_1',\dots,x_n';g_0,m_0,\epsilon) \end{aligned} \tag{21.21}$$

become finite after being renormalized by the inverse factors ${Z_\phi}^{-n/2}(g,\varepsilon)$ of (21.20):

$$\Gamma^{(n)}(x_1,\dots,x_n;g,m,\mu)={Z_\phi}^{-n/2}{\Gamma_0}^{(n)}(x_1,\dots,x_n;g_0,m_0,\epsilon). \tag{21.22}$$

As discussed in Chapter 9, there are different possible methods of fixing the counterterms. The most common choice is based on the normalization conditions

$$\frac{\partial}{\partial p^2}\Gamma^{(2)}|_{p^2=-\mu^2} = 1, \tag{21.23}$$

$$\Gamma^{(2)}|_{p^2=-\mu^2} = m^2, \tag{21.24}$$

$$\Gamma^{(4)}|_{\text{symm point}} = \mu^\epsilon. \tag{21.25}$$

where the symmetry point is defined by

$$p_ip_j=-\frac{\mu^2}{4}(4\delta_{ij}-1);\quad i,j=1,\dots,4. \tag{21.26}$$

The *minimal subtraction scheme* due to 't Hooft requires, instead, the cancellation of all $1/\epsilon, 1/\epsilon^2, 1/\epsilon^3,\dots$ pole terms in the vertex functions. This has the pleasant property that the resulting counterterms depend only on the coupling constants and not on the mass m.

In both schemes, the arbitrary mass parameter μ can be avoided by setting it equal to m of the fields are massive, but is unavoidable in massless theories.

21.3 The Renormalization Group Equation

As discussed above, physical observables should be independent on choice of μ, and this fundamental property will now be formulated quantitatively. Suppose we calculate perturbatively the bare n-point vertex function at a fixed bare coupling g_0 and mass m_0 the bare vertices in $4-\epsilon$ dimensions:

$$\Gamma_0^{(n)}(p_1,\dots,p_n;g_0,m_0,\epsilon). \tag{21.27}$$

The result is trivially independent of the choice of the mass parameter μ which was introduced only to define the finite renormalized coupling strength $g=g(\mu)$ and mass $m=m(\mu)$. We therefore have the obvious relation

$$\mu\frac{\partial}{\partial\mu}\Gamma_0^{(n)}(p_1,\dots p_n;g_0,m_0,\epsilon)=0, \tag{21.28}$$

This obvious relation turns into a nontrivial one for the renormalized vertex functions

$$\Gamma^{(n)}(p_1,\dots,p_n;g,m,\mu)\equiv Z_\phi^{-n/2}(g_0,m_0,\epsilon)\Gamma_0^{(n)}(p_1,\dots,p_n;g_0,m_0,\epsilon). \tag{21.29}$$

If the bare parameters g_0,m_0,ϵ are kept fixed, the μ dependence in $\Gamma^{(n)}$ can come from the renormalized quantities g and m whose values epend on the choice of μ, which is emphasized by writing them as $g(\mu)$ and $m(\mu)$. By applying (21.28) to (21.29) we see from the chain rule of differentiation that

$$\begin{aligned}\left(\mu\partial_\mu + \mu\partial_\mu g|_{g_0,m_0,\epsilon} - n\mu\partial_\mu \log Z_\phi^{1/2}|_{g_0,m_0,\epsilon} + \mu\partial_\mu \log m^2|_{g_0,m_0,\epsilon} m^2\partial_{m^2}\right)& \\ \times\Gamma^{(n)}(p_1,\dots,p_n;g,m,\mu) = 0,& \qquad (21.30)\end{aligned}$$

where we have written ∂_μ for $\partial/\partial\mu$, to save space. The right-hand sides of (21.30) (21.30) can be expressed as finite functions of g, m, and μ. One defines the functions

$$\beta = \mu\partial_\mu g|_{g_0,m_0,\epsilon}, \qquad (21.31)$$

$$\gamma = \mu\partial_\mu \log Z_\phi^{1/2}|_{g_0,m_0,\epsilon}, \qquad (21.32)$$

$$\gamma_{m^2} = \mu\partial_\mu \log m^2|_{g_0,m_0,\epsilon\cdot}, \qquad (21.33)$$

and reexpressed them as functions of g, m, and μ. With these, Eq.(21.31) becomes the following differential equation

$$(\mu\partial_\mu + \beta\partial_g - n\gamma + \gamma_{m^2}m^2\partial_{m^2})\Gamma^{(n)}(p_1,\dots,p_n;g,m,\mu) = 0. \qquad (21.34)$$

This is the celebrated *renormalization group equation*(RGE) If we would not use the minimal subtraction scheme but some cutoff Λ in momentum space, then the parameter ϵ in Eqs.(21.27) (21.33) would be replaced by the cutoff Λ. The RGE is the quantitative formulation of the invariance of the vertex functions $\Gamma^{(n)}$ under a change of the auxiliary mass scale μ, which on the one hand appears explicitly in the vertex functions $\Gamma^{(n)}(p_1,\dots,p_n;g,m,\mu)$, on the other hand in the μ-dependent renormalized quantities $g = g(\mu)$ and $m = m(\mu)$.

21.4 Calculation of Coefficient Functions from Counter Terms

The solution of a partial differential equation like (21.34) is, in general, awkward, since $\beta, \gamma, \gamma_{m^2}$ may depend on g, m and μ. It is an important special property of t'Hooft's renormalization scheme, that the counterterms c^g, c^{m^2}, and c^ϕ happen to be independent of the masses m and depend only on the coupling constant g, apart from ϵ. This makes their calculation simple and, moreover, produces coefficient functions $\beta, \gamma, \gamma_{m^2}$ in the RGE (21.34) which depend only on g and ϵ. Suppressing the ϵ-argument, we shall therefore write $\beta(g), \gamma(g), \gamma_{m^2}(g)$.

Consider first $\gamma(g)$. Since Z_ϕ depends only on g we certainly have

$$\gamma(g) = \mu\partial_\mu g|_{g_0,m_0,\epsilon} \cdot \frac{d}{dg}\log Z_\phi^{1/2}(g).$$

With the help of (21.31), this can be rewritten as

$$\gamma(g) = \beta(g)\frac{d}{dg}\log Z_\phi^{1/2}(g). \qquad (21.35)$$

Similarly, using the renormalization equation $m^{-2} = m_0^{-2}\bar{Z}_m(g)Z_\phi^{-1}(g)$ we see that

$$\gamma_{m^2}(g) = -\beta(g)\left(\frac{d}{dg}\log\bar{Z}_m - \frac{d}{dg}\log Z_\phi\right) \tag{21.36}$$

or

$$\gamma_{m^2}(g) - 2\gamma(g) \equiv \bar{\gamma}_{m^2}(g) = -\beta(g)\frac{d}{dg}\log\bar{Z}_m(g). \tag{21.37}$$

Finally, we use

$$g_0 = g\mu^\epsilon\bar{Z}_g(g)Z_\phi^{-2}(g) \tag{21.38}$$

to find

$$\begin{aligned}\beta(g) &= \frac{-\mu\partial_\mu g_0|_g}{\partial_g g_0|_\mu} = -\epsilon\left[\frac{d}{dg}\log(g\bar{Z}_g Z_\phi^{-2})\right]^{-1}\\ &= -\frac{\epsilon g}{1+g[\log(g\bar{Z}_g)]' - 2g[\log(\bar{Z}_\phi)]'}.\end{aligned} \tag{21.39}$$

or, using (21.35),

$$\beta(g) = \frac{-\epsilon + 4\gamma(g)}{\log[g\bar{Z}_g(g)]'} \tag{21.40}$$

All three functions depend only on g.

The formulas can be brought to a more practical shape by making use of the explicit $1/\epsilon$-expansion structure of the counterterms as functions of g. Then we may rewrite Eqs. (21.35), (21.37), (21.40) as follows

$$\gamma(g)\left(1+\sum_{\nu=1}^{\infty}c_\nu^\phi(g)\epsilon^{-\nu}\right) = \frac{1}{2}\beta(g)\sum_{\nu=1}^{\infty}c_\nu^\phi(g)'\epsilon^{-\nu}, \tag{21.41}$$

$$[-\gamma_{m^2}(g)+2\gamma(g)]\left(1+\sum_{\nu=1}^{\infty}c_\nu^m(g)\epsilon^{-\nu}\right) = \beta(g)\sum_{\nu=1}^{\infty}c_\nu^m(g)'\epsilon^{-\nu}, \tag{21.42}$$

$$\beta(g)\left(\sum_{\nu=1}^{\infty}[gc_\nu^g(g)]'\epsilon^{-\nu}\right) = [-\epsilon+4\gamma(g)]g\left(1+\sum_{\nu=1}^{\infty}c_\nu^g(g)\epsilon^{-\nu}\right). \tag{21.43}$$

For a renormalizable theory, the functions $\beta(g)$, $\gamma(g)$, $\gamma_{m^2}(g)$ have to remain finite in the limit $\epsilon \to 0$. Thus we can expand these quantities in a power series in ϵ with powers ϵ^0, ϵ^1, ϵ^2 .... By inserting (21.41) into (21.43) we see that $\beta(g)$ can at most contain the following powers of ϵ:

$$\beta(g) = \beta_0(g) + \epsilon\beta_1(g). \tag{21.44}$$

When inserting this into (21.41), (21.42), we find $\gamma(g)$ and $\gamma_{m^2}(g)$ to be independent of ϵ. Equating the regular parts of the three equations yields

$$\begin{aligned}\beta_0+\epsilon\beta_1+\beta_1(c_1^g+gc_1^{g\prime}) &= (-\epsilon+4\gamma)g-gc_1^g\\ \gamma &= \frac{1}{2}\beta_1c_1^{\phi\prime}\\ \bar\gamma_{m^2} &\equiv \gamma_{m^2}-2\gamma=-\beta_1c_1^{m\prime}\end{aligned}\qquad(21.45)$$

which are solved by

$$\begin{aligned}\beta_1(g) &= -g\\ \beta_0(g) &= g^2c_1^g(g)'+4\gamma g\end{aligned}\qquad(21.46)$$

Thus, amazingly, the three functions $\beta(g),\gamma(g),\gamma_{m^2}(g)$ can be expressed in terms of g-derivatives of the three residues $c_1^g(g)$, $c_1^\phi(g)$, $c_1^m(g)$ of the simple $1/\epsilon$-poles in the counterterms:

$$\begin{aligned}\beta(g)=-\epsilon g+g^2c_1^g(g)'+4\gamma g,\\ \gamma(g)=-\frac{g}{2}c_1^\phi(g)',\\ \bar\gamma_{m^2}(g)=\gamma_{m^2}(g)-2\gamma(g)=gc_1^m(g)'.\end{aligned}\qquad(21.47)$$

The finiteness of $\beta(g),\gamma(g),\gamma_{m^2}(g)$ at $\epsilon=0$ forces all higher residues of in Eqs. (21.41) (21.43) to disappear. This implies an infinite set of consistency relations among the expansion coefficients which are useful for checking the calculations:

$$\beta_0(gc_\nu^g)'-g(gc_{\nu+1}^g)' = 4\gamma gc_\nu^g g-c_{\nu+1}^g,\qquad(21.48)$$

$$\gamma c_\nu^\phi = \beta_0c_\nu^{\phi\prime}-gc_{\nu+1}^{\phi}{}',\qquad(21.49)$$

$$(\gamma_{m^2}-2\gamma)c_\nu^m = -\beta_0c_\nu^{m\prime}+gc_{\nu+1}^{m}{}'.\qquad(21.50)$$

Let us now turn to the actual calculation of $\beta(g),\gamma(g),\gamma_{m^2}(g)$ in the O(N)-symmetric ϕ^4 theory. The renormalization constants were given in Section 9.7. Replacing $g\bar{S}_D$ by g, for brevity (so that it becomes equal to our former λ) we obtained [recall Eqs. (9.243)]

$$\begin{aligned}\bar Z_g &= 1+c^g=1+g\frac{3}{2}T_I\frac{1}{\epsilon}+g^2\left\{\frac{15}{4}T_{I^2}\frac{1}{\epsilon^2}-3T_{I_4}\left(\frac{1}{2\epsilon^2}+\frac{1}{4\epsilon}\right)\right\},\\ Z_\phi &= 1+c^\phi=1-g^2\frac{1}{48}T_{D_3}\frac{1}{\epsilon},\\ \bar Z_m &= 1+c^m=1+g\frac{1}{2}T_{D_1}\frac{1}{\epsilon}+\frac{g^2}{4}\left\{3T_{D_1D_2}\frac{1}{\epsilon^2}-T_{D_3}\left(\frac{1}{\epsilon^2}+\frac{1}{2\epsilon}\right)\right\}.\end{aligned}\qquad(21.51)$$

The $1/\epsilon$-pole terms are

$$\begin{aligned}c_1^g &= g\frac{3}{2}T_I-g^2\frac{3}{4}T_{I_4},\\ c_1^\phi &= -g^2\frac{1}{48}T_{D_3},\\ c_1^{m^2} &= g\frac{1}{2}T_{D_1}-g^2\frac{1}{8}T_{D_3}.\end{aligned}\qquad(21.52)$$

Inserting these into (21.47), we find

$$\begin{aligned}\beta(g)-4\gamma(g)g &= -\epsilon g+\frac{3}{2}g^2T_I-\frac{3}{2}g^3T_{I_4},\\ \gamma(g) &= g^2\frac{1}{48}T_{D_3},\\ \gamma_{m^2}(g)-2\gamma(g) &= \frac{g}{2}T_{D_1}-\frac{g^2}{4}T_{D_3}.\end{aligned}\tag{21.53}$$

The reduced matrix elements T were given in (5.75). For $N=1$, all T's are equal to unity.

Explicitly, we can solve for $\beta(g),\gamma(g),\gamma_{m^2}(g)$ as follows [making use of the explicit reduced matrix elements T calculated in Eqs. (9.228) (9.240).

$$\begin{aligned}\beta(g) &= -\epsilon g+g^2\frac{3}{2}T_I-g^3\left(\frac{3}{2}T_{I_4}-\frac{1}{12}T_{D_3}\right)\\ &= -\epsilon g+\frac{N+8}{6}g^2-\frac{3N+14}{12}g^3,\end{aligned}\tag{21.54}$$

$$\gamma(g) = g^2\frac{1}{48}T_{D_3}=g^2\frac{1}{48}\frac{N+2}{3},\tag{21.55}$$

$$\gamma_{m^2}(g) = g\frac{1}{2}T_{D_1}-g^2\frac{5}{24}T_{D_3}=\left(g\frac{1}{2}-g^2\frac{5}{24}\right)\frac{N+2}{3}.\tag{21.56}$$

With the help of Eqs. (21.48) (21.50) we check these results for consistency:

$$\begin{aligned}\beta_0(gc_1^g)'-g(gc_2^g)' &= 4\gamma gc_1{}^g-gc_2{}^g,\\ \gamma c_1^\phi &= \beta_0c_1^{\phi\prime}-gc_2^{\phi\prime},\\ (\gamma_{m^2}-2\gamma)c_1^m &= -\beta_0c_1^{m\prime}+gc_2^{m\prime}.\end{aligned}\tag{21.57}$$

Inserting (21.54) (21.56), we see that to order g^2, the two sides are indeed equal.

It is instructive to observe the cancellation of $1/\epsilon^n$-singularities in Eqs. (21.35) (21.40) a somewhat more explicitly. Take for instance $\gamma(g)$ of Eq. (21.35), and the five-loop result for the β-function to be stated in (21.192) for $N=1$:

$$\begin{aligned}\beta(g) &= -\epsilon g+\frac{3}{2}g^2-\frac{17}{12}g^3+\left[\frac{145}{64}+\frac{3\zeta(3)}{2}\right]g^4\\ &+\left[-\frac{3499}{768}+\frac{\pi^4}{80}-\frac{39\zeta(3)}{8}-\frac{15\zeta(5)}{2}\right]g^5+\\ &+\left[\frac{764621}{73728}-\frac{1189\pi^4}{23040}-\frac{5\pi^6}{448}+\frac{7965\zeta(3)}{512}+\frac{45\zeta(3)^2}{32}+\frac{987\zeta(5)}{32}+\frac{1323\zeta(7)}{32}\right]g^6.\end{aligned}\tag{21.58}$$

The logarithmic derivative of the renormalization constant has the five-loop expansion:

$$[\log Z_\phi(g)]' = -\frac{1}{24\epsilon}g-\left(\frac{1}{16\epsilon^2}-\frac{1}{64\epsilon}\right)g^2+\left(-\frac{3}{32\epsilon^3}+\frac{95}{1152\epsilon^2}-\frac{65}{1536\epsilon}\right)g^3$$

$$+\left[-\frac{9}{64\epsilon^4}+\frac{163}{768\epsilon^3}-\frac{553}{3072\epsilon^2}+\frac{3709}{36864\epsilon}+\frac{\pi^4}{2880\epsilon}-\frac{\zeta(3)}{16\epsilon^2}-3\frac{\zeta(3)}{256\epsilon}\right]g^4 \tag{21.59}$$
$$+\left[-\frac{13}{3072\epsilon^4}+\frac{179}{55296\epsilon^3}-\frac{23}{16384\epsilon^2}\right]g^5$$

When forming the product $\beta(g)\cdot[\log Z_\phi(g)]'$ to get $\gamma(g)$ via (21.35), the only ϵ-term in $\beta(g)$ reduces the highest $1/\epsilon^n$ singularities in the g^n-term of $[\log Z_\phi(g)]'$ by one power of $1/\epsilon$. For $n \geq 2$ the resulting terms are still singular, but they are canceled by the product of the finite g^2-term in $\beta(g)$ and the singular terms associated with the lower power g^{n-1} in $[\log Z_\phi(g)]'$, etc..

21.5 Solution of Renormalization Group Equations for Vertex Functions

The subtraction of divergencies via the ϵ-expansion has given us coefficient functions $\beta, \gamma, \gamma_{m^2}$ which depend only on the renormalized coupling constant $g(\mu)$. This makes it easy to solve the renormalization group equation (21.34). Suppose we have calculated the renormalized vertex functions for some initial mass scale μ with a renormalized coupling $g = g(\mu)$ and mass $m = m(\mu)$. Then the coupling $g(\mu') = g(\sigma\mu)$ at an arbitrary mass scale $\mu' = \sigma\mu$, which we shall denote for brevity by $\equiv g_\sigma$, is given by

$$\sigma\frac{d}{d\sigma}g_\sigma = \beta(g_\sigma). \tag{21.60}$$

Equation (21.60) can be rewritten as

$$\frac{d\ln\sigma}{dg_\sigma} = \frac{1}{\beta(g_\sigma)} \tag{21.61}$$

This is solved with the initial condition

$$g_1 = g. \tag{21.62}$$

The result is

$$\ln\sigma = \int_g^{g_\sigma}\frac{dg'}{\beta(g')}. \tag{21.63}$$

Similarly we have for the μ-dependence of the renormalized mass $m(\mu)$ the equation

$$m^{-2}(\mu)\mu\frac{d}{d\mu}m^2(\mu) = \gamma_{m^2}(g_\sigma), \tag{21.64}$$

which can be rewritten as with the notation $m_\sigma \equiv m(\sigma\mu) = m(\mu')$ as

$$\frac{d\ln m_\sigma^2}{d\ln\sigma} = \gamma_{m^2}(g_\sigma), \tag{21.65}$$

and is solved with the initial condition

$$m_1 = m \tag{21.66}$$

by

$$\ln \frac{m_\sigma^2}{m^2} = \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma_{m^2}(g_{\sigma'}). \tag{21.67}$$

Using the functions g_σ and m_σ, the renormalization group equation for the vertex functions which is initially a partial differential equation can be rephrased as an ordinary differential equation:

$$\left[\sigma \frac{d}{d\sigma} - n\gamma(g_\sigma)\right] \Gamma^{(n)}(p_i; g_\sigma, m_\sigma, \sigma\mu) = 0. \tag{21.68}$$

For brevity, we have written p_i collectively for $p_1, \ldots, p_n$. Equation (21.68) is immediately integrated as follows

$$\Gamma^{(n)}(p_i; g_\sigma, m_\sigma, \sigma\mu) \;=\; \exp\left[n \int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma(g_{\sigma'})\right] \Gamma^{(n)}(p_i; g, m, \mu), \tag{21.69}$$

which shows the full σ-dependence of the renormalized vertex functions.

This equation can now be used to study the critical behavior of $\Gamma^{(n)}(p_i; g, m, \mu)$, i.e.,the behavior of $\Gamma^{(n)}$ as the renormalized mass m goes to zero while the mass scale μ at which the theory is defined remains fixed. For this purpose it is useful to take advantage of the dimensional structure of the vertex functions. In D dimensions, a field has a (mass) dimension $d_\phi = D/2 - 1$. A Green function containing n fields has the dimension $d_\varphi = n(D/2 - 1)$. When performing $n - 1$ Fourier transforms of the fields to momentum space, $\int d^D x e^{ipx}$, the dimension becomes $nd_\varphi - (n-1)D$. The Fourier transformed two-point function $G^{(2)}(p)$ has dimension -2 for all D. The vertex function $\Gamma^{(n)}$ is obtained by multiplying the Fourier transformed Green function $G^{(n)}$ by n factors $G^{(2)}(p)^{-1}$. The total mass dimension of $\Gamma^{(n)}$ is therefore $D - nd_\varphi = D - n(D/2-1)$. Then, since the dimension of p_i, g, m, μ are 1, 0, 1, 1, respectively, the vertex function $\Gamma^{(n)}$ must satisfy the trivial identity valid for any scale parameter σ,

$$\Gamma^{(n)}\left(p_i; g, m, \mu\right) = \sigma^{D - \frac{n}{2}(D-2)} \Gamma^{(n)}\left(p_i/\sigma;\; g,\; m/\sigma,\; \mu/\sigma\right). \tag{21.70}$$

Inserting on the right-hand side the left-hand side of (21.69), we obtain

$$\Gamma^{(n)}(p_i; g, m, \mu) = \sigma^{D-n(D/2-1)} \exp\left[-n \int_1^\sigma d\sigma' \frac{\gamma(g_{\sigma'})}{\sigma'}\right] \Gamma^{(n)}\left(p_i/\sigma, g_\sigma, m_\sigma/\sigma, \mu\right). \tag{21.71}$$

We now choose $\sigma = \sigma_m$ so that the rescaled mass m_σ/σ is equal to the mass parameter μ:

$$m_\sigma/\sigma|_{\sigma=\sigma_m} = \mu. \tag{21.72}$$

Then (21.71) becomes

$$\Gamma^{(n)}(p_i; g, m, \mu) = \sigma_m^{D-n(D/2-1)} \exp\left[-n \int_1^{\sigma_m} d\sigma' \frac{\gamma(g_{\sigma'})}{\sigma'}\right] \Gamma^{(n)}\left(p_i/\sigma_m, g_{\sigma_m}, \mu, \mu\right). \tag{21.73}$$

This equation relates the renormalized vertex functions $\Gamma^{(n)}(p_i, g, m, \mu)$ of an arbitrary mass to those of a fixed mass equal to the mass parameter μ at rescaled momenta p_i/σ and a running coupling constant coupling constant g_σ. Apart from a trivial overall rescaling factor $\sigma_m^{D-n(D/2-1)}$ due to the naive dimension, there is also a nontrivial exponential function.

Explicitly, the parameter σ_m in (21.72) is found by using Eq. (21.67) to calculate the ratio

$$\begin{aligned}
\frac{m^2}{\mu^2} &= \frac{m_\sigma^2}{\mu^2}\exp\left\{\int_0^{\sigma_m}\frac{d\sigma'}{\sigma'}\left[-\gamma_{m^2}(g_{\sigma'})\right]\right\}. \\
&= \frac{m_\sigma^2}{\sigma^2\mu^2}\exp\left\{\int_0^{\sigma_m}\frac{d\sigma'}{\sigma'}\left[2-\gamma_{m^2}(g_{\sigma'})\right]\right\} \\
&= \exp\left\{\int_0^{\sigma_m}\frac{d\sigma'}{\sigma'}\left[2-\gamma_{m^2}(g_{\sigma'})\right]\right\}. \qquad (21.74)
\end{aligned}$$

Our goal is to study the behavior of the vertex functions on the left-hand side of (21.73) in the critical region where $m \to 0$. On the right-hand side, the mass dependence resides in the rescaling parameter σ_m.

In many-body systems undergoing a second-order phase transition, the mass m approaches zero proportional to $T - T_c$. Equation (21.74) specifies how the auxiliary scale parameter σ_m which rules the scaling relation (21.73) behaves for $T \to T_c$.

Near the critical point $T = T_c$, experimental correlation functions show a simple scaling behavior. Such a behavior can be found from Eqs. (21.73) and (21.74), if in the limit $m \to 0$ the coupling constant g runs into a *fixed point* $g^\star$, at which the running coupling constant g_σ becomes independent of σ, i.e.,

$$\left[\frac{dg_\sigma}{d\sigma}\right]_{g=g^\star} = 0, \qquad (21.75)$$

Assuming that $\gamma^*_{m^2} \equiv \gamma_{m^2}(g^*) < 2$, which will be true in the present field theory, the integrand in Eq. (21.74) is singular at $\sigma = 0$, and the asymptotic behavior of σ_m for $m \to 0$ can immediately be found:

$$\frac{m^2}{\mu^2} \overset{m\approx 0}{\approx} \exp\left\{\int_0^{\sigma_m}\frac{d\sigma'}{\sigma'}\left[2-\gamma_{m^2}(g^*)\right]\right\} = \sigma_m^{2-\gamma^*_{m^2}}. \qquad (21.76)$$

we see that σ_m goes to zero for $m \to 0$ with the power law

$$\sigma_m \approx \left(\frac{m^2}{\mu^2}\right)^{1/(2-\gamma^*_{m^2})}. \qquad (21.77)$$

In applications to second-order phase transitions we shall identify m^2/μ^2 with the relative distance from the critical temperature

$$\frac{m^2}{\mu^2} \equiv \tau \equiv \frac{T - T_c}{T_c}, \qquad (21.78)$$

and write (21.77) as

$$\sigma_m \approx \tau^{1/(2-\gamma^*_{m^2})} \tag{21.79}$$

In this limit, the exponential prefactor in (21.73) has the power behavior

$$\exp\left[-n\int_1^{\sigma_m}\frac{d\sigma'}{\sigma'}\gamma(g_{\sigma'})\right] \overset{\sigma_m\approx 0}{\approx} \tau^{n\gamma^*/(2-\gamma^*_{m^2})}. \tag{21.80}$$

where $\gamma^* \equiv \gamma(g^*)$. The n-point vertex function behaves therefore like

$$\Gamma^{(n)}(p_i; g, m, \mu) \overset{m\approx 0}{\approx} \sigma_m^{D-n(D/2-1)-n\gamma^*}\,\Gamma^{(n)}(p_i/\sigma_m; g^*, \mu, \mu). \tag{21.81}$$

For the two-point vertex function this implies a momentum dependence

$$\Gamma(p; g, m, \mu) \overset{m\approx 0}{\approx} p^{2-2\gamma^*}\tilde{f}(p/\sigma_m). \tag{21.82}$$

with some function $\tilde{f}(\kappa)$. When going over to the two-point function in x-space

$$G(\mathbf{x}; g, m, \mu) = \int\frac{d^Dp}{(2\pi)^D}e^{i\mathbf{px}}\frac{1}{\Gamma(p; g, m, \mu)} \tag{21.83}$$

this amounts to an x-dependence

$$G(\mathbf{x}; g, m, \mu) \overset{m\approx 0}{\approx} \frac{1}{r^{D-2+2\gamma^*}}\tilde{g}(\mathbf{x}/\sigma_m) = \frac{1}{r^{D-2+2\gamma^*}}\tilde{g}\left(\mathbf{x}(m^2/\mu^2)^{1/(2-\gamma^*_{m^2})}\right). \tag{21.84}$$

This is of a general form discovered by Kadanoff fpr connected correlation functions:

$$G_{\rm c}^{(2)}(\mathrm{r}) = \frac{f(r/t^{-\nu})}{r^{D-2+\eta}}, \tag{21.85}$$

With the identification (21.78, we see that the critical exponent ν in (21.85) is given by

$$\nu = \frac{1}{2-\gamma^*_{m^2}}. \tag{21.86}$$

For $T \rightarrow T_c$, the length scale $\xi =$ diverges like

$$\xi(t) = \xi_0\,|t|^{-\nu}. \tag{21.87}$$

By comparing the power behavior at the critical point in (21.84) with that in (21.85) we identify the critical exponent η as

$$\eta = 2\gamma^* : \tag{21.88}$$

21.6 Renormalization Group for Effective Action and Potential

The same methods can be applied to find the one parameter set of identical theories for the full effective action $\Gamma[\Phi]$ for different values of the mass parameter μ. Consider the power series expansion of the effective action in terms of vertex functions

$$\Gamma[\Phi; g, m, \mu] = \sum_{n=0}^{\infty} \frac{1}{n!} \int \frac{d^D p_1}{(2\pi)^D} \cdots \frac{d^D p}{(2\pi)^D} \Phi(p_1) \cdots \Phi(p_n) \Gamma^{(n)}(p_1, \ldots, p_n; g, m, \mu). \tag{21.89}$$

and apply the RGE in Eq.(21.34) to every coefficient. This effectively replaces the factor n in front of $\gamma(g)$ as follows

$$n \longrightarrow \int \frac{d^D p}{(2\pi)^D} \Phi(p) \frac{\delta}{\delta\Phi(p)}. \tag{21.90}$$

Hence we find immediately the RGE

$$\left[\mu\partial_\mu + \beta(g)\partial_g - \gamma(g) \int \frac{d^D p}{(2\pi)^D} \Phi(p) \frac{\delta}{\delta\Phi(p)} + \gamma_{m^2}(g) m^2 \partial_{m^2}\right] \Gamma[\Phi; g, m, \mu] = 0. \tag{21.91}$$

A corresponding result holds for the effective potential

$$v(\Phi) = -L^{-D} \Gamma[\Phi; g, m, \mu]|_{\Phi(x)=\text{const}=\Phi}, \tag{21.92}$$

where L is the size of the D-dimensional box under consideration. The effective potential satisfies the differential equation

$$\left[\mu\partial_\mu + \beta(g)\partial_g - \gamma(g)\Phi \frac{\partial}{\partial\Phi} + \gamma_{m^2}(g) m^2 \partial_{m^2}\right] v(\Phi; g, m, \mu) = 0. \tag{21.93}$$

Because of its relevance to physical applications we shall first solve only this latter equation along the lines of Eqs.(21.63) (21.68). We introduce an additional running field strength $\Phi(\sigma)$ satisfying the differential equation

$$\frac{1}{\Phi(\sigma)} \sigma \frac{d}{d\sigma} \Phi(\sigma) = -\gamma(g(\sigma)), \tag{21.94}$$

with the initial condition

$$\Phi(1) = \Phi. \tag{21.95}$$

This is solved by

$$\frac{\Phi(\sigma)}{\Phi} = \exp\left[-\int_1^\sigma \frac{d\sigma'}{\sigma'} \gamma(g'_\sigma)\right]. \tag{21.96}$$

Using Φ_σ, we have the identity along the renormalization trajectory

$$v(\Phi; g_\sigma, m_\sigma, \sigma\mu) \equiv v(\Phi; g, m, \mu). \tag{21.97}$$

Note that there is no prefactor in contrast to (21.73). All m-dependence is contained in m_σ and $\Phi(\sigma)$ via (21.96). In the limit $\sigma \to 0$ the field behaves like

$$\frac{\Phi(\sigma)}{\Phi} \approx \sigma^{-\gamma^*}. \tag{21.98}$$

Since $\Gamma[\Phi]$ is dimensionless and $v(\Phi)$ is related to $\Gamma[\Phi]$ by (21.92), the dimensional transformation corresponding to (21.70) becomes simply

$$v(\Phi; g, m, \mu) = \sigma^D v(\Phi/\sigma^{D/2-1}; g, m/\sigma, \mu/\sigma) \tag{21.99}$$

Combining this with (21.97), we find

$$v(\Phi; g, m, \mu) = \sigma^D v(\Phi_\sigma/\sigma^{D/2-1}, g, m_\sigma/\sigma, \mu). \tag{21.100}$$

At the mass-dependent value σ_m of Eq. (21.72), we obtain the analog of (21.73) for the effective potential

$$v(\Phi; g, m, \mu) = \sigma_m^D v(\Phi_{\sigma_m}/\sigma_m^{D/2-1}; g_{\sigma_m}, \mu, \mu). \tag{21.101}$$

In the critical regime, where $\sigma \to 0$, Eq. (21.96) becomes

$$\frac{\Phi_{\sigma_m}}{\Phi} \approx \sigma_m^{-\gamma^*}, \tag{21.102}$$

and the effective potential has the power behavior

$$v(\Phi; g, m, \mu) \overset{m\approx 0}{\approx} \sigma_m^D\, v(\Phi/\sigma_m^{\gamma^*+D/2-1}; g^*, \mu, \mu). \tag{21.103}$$

this goes over onto For applications to systems below T_c it is most convenient to consider, instead of $\Gamma[\Phi; g, m, \mu]$, the vertex functions in the presence of an external magentization. They are obtained by expanding $\Gamma[\Phi; g, m, \mu]$ functionally around $\Phi(x) \equiv \Phi_0$:

$$\Gamma^{(n)}(p_1, \dots, p_n; \Phi_0, m, \mu) \equiv \frac{\delta^n}{\delta\Phi(x_1)\dots\delta\Phi(x_n)}\Gamma[\Phi; g, m, \mu]|_{\Phi\equiv\Phi_0}. \tag{21.104}$$

This gives

$$\Gamma^{(n)}(p_1, \dots, p_n; \Phi_0, g, m, \mu) = \sum_{n'=0}^{\infty} \frac{\Phi_0^{n+n'}}{n'!}\Gamma^{(n+n')}(p_1, \dots p_n, 0, \dots, 0; g, m, \mu), \tag{21.105}$$

where the zeros later the arents $p_1, \dots, p_n$ indicate that there are n' more momentum arents $p_{n+1}, \dots, p_{n+n'}$ which have been set zero since each constant field Φ_0 has a momentum dependence $\delta^{(D)}(p)\Phi_0$. Thus the renormalization group equation for the vertex function at a non-zero field, $\Gamma^{(n)}(p_1,\dots,p_n;\Phi_0,,\mu)$, can be obtained from those at zero field $\Gamma^{(n+n')}(p_1,\dots p_n,p_{n+1},\dots,p_{n+n'};\mu)$ with the last n' momenta set equal to zero, i.e., from

$$\left[\mu\partial_\mu+\beta(g)\partial_g-(n+n')\gamma(g)+\gamma_{m^2}(g)m^2\partial_{m^2}\right]\Gamma^{(n+n')}(p_1,\dots,p_n,0,\dots 0;g,m,\mu)=0. \tag{21.106}$$

Inserting these equations into (21.105), we obtain the RGE

$$\left[\mu\partial_\mu+\beta(g)\partial_g-\gamma(g)\left(\Phi_0\frac{\partial}{\partial\Phi_0}\right)+\gamma_{m^2}(g)m^2\partial_{m^2}\right]\Gamma^{(n)}(p_1,\dots,p_n;\Phi_0,g,m,\mu)=0. \tag{21.107}$$

When treated as above, this leads to the scaling relation

$$\Gamma^{(n)}(p_i;\Phi_0,g,m,\mu)=e^{-n\int_1^\sigma\frac{d\sigma'}{\sigma'}\gamma(g_{\sigma'})}\Gamma^{(n)}(p_i;\Phi_{0\,\sigma},g_\sigma,m_\sigma,\mu\sigma) \tag{21.108}$$

Together with the trivial scaling relation check

$$\Gamma^{(n)}(p_i;\Phi_0,g,m,\mu)=\sigma^{D-n(D/2-1)}\Gamma^{(n)}(p_i/\sigma;\Phi_0/\sigma^{D/2-1},g,m/\sigma,\mu/\sigma), \tag{21.109}$$

we find

$$\begin{aligned}\Gamma^{(n)}(p_i;\Phi_0,g,m,\mu) &= \sigma^{D-n(D/2-1)}e^{-n\int_1^\sigma\frac{d\sigma'}{\sigma'}\gamma(g_{\sigma'})}\\ &\quad\times\Gamma^{(n)}(p_i/\sigma;\Phi_{0\,\sigma}/\sigma^{D/2-1},g_\sigma,m_\sigma/\sigma,\mu),\end{aligned} \tag{21.110}$$

which becomes at $\sigma=\sigma_m$ of Eq. (21.72):

$$\begin{aligned}\Gamma^{(n)}(p_i;\Phi_0,g,m,\mu) &= \sigma_m^{D-n(D/2-1)}e^{-n\int_1^{\sigma_m}\frac{d\sigma'}{\sigma'}\gamma(g_{\sigma'})}\\ &\quad\times\Gamma^{(n)}(p_i/\sigma_m;\Phi_{0\,\sigma_m}/\sigma_m^{D/2-1},g_{\sigma_m},\mu,\mu),\end{aligned} \tag{21.111}$$

and thus, near the critical point,

$$\Gamma^{(n)}(p_i;\Phi_0,g,m,\mu)=\sigma_m^{D-n(\gamma^*+D/2-1)}\Gamma^{(n)}(p_i/\sigma_m;\Phi_0/\sigma_m^{\gamma^*+D/2-1},g^*,\mu,\mu). \tag{21.112}$$

21.7 Approach to Scaling

In Eq. (21.84) we have extracted from the scaling relation (21.81) for the two-point vertex function Kadanoff's scaling law (21.85). From this we read off the critical exponents $\nu=1/(2-\gamma_m^*)$ for the temperature nehavior of the coherence length and the exponent $\eta=2\gamma^*$ for the critical power behavior of the green function.

There exists a further important critical exponent which governs the approach to the scaling law (21.84). In order to find this we expand the right-hand side of Eq. (21.73) around g^* and write

$$\begin{aligned}\Gamma^{(n)}(p_i;g,m,\mu) &= \sigma_m^{D-n(D/2-1)}\exp\left[-n\int_1^{\sigma_m}d\sigma'\frac{\gamma(g_{\sigma'})}{\sigma'}\right]\Gamma^{(n)}\left(p_i/\sigma_m,g^*,\mu,\mu\right).\\ &\quad\times C^{(n)}(p_i/\sigma_m;g_{\sigma_m},\mu,\mu)\end{aligned} \tag{21.113}$$

Using Eq. (21.7), we obtain the correction factor

$$C^{(n)}(p_i;\sigma_m,g^*,\mu,\mu)=1+[g_{\sigma_m}-g^*]\psi^{(n)}(p_i/\sigma_m;g^*,\mu,\mu)+\dots\,. \tag{21.114}$$

where $\psi^{(n)}$ is th dimensionless function

$$\psi^{(n)}(p_i/\sigma_m;g^*,\mu,\mu)=\frac{\partial}{\partial g}\log\Gamma^{(n)}(p_i/\sigma_m;g^*,\mu,\mu). \tag{21.115}$$

The way in which $g(\sigma)$ tends to g^* when approaching the critical point can readily be deduced from Eq. (21.63). Let ω be the slope of the β-function at the zero:

$$\omega\equiv\left.\frac{d\beta(g)}{dg}\right|_{g=g^*}. \tag{21.116}$$

Then we can expand near g^*

$$\beta(g)=\omega(g-g^*)+\mathcal{O}((g-g^*)^2), \tag{21.117}$$

and deduce from (21.63) the behavior

$$\log\sigma\approx\frac{1}{\omega}\log(g_\sigma-g^*)+\dots\,, \tag{21.118}$$

implying for small m the approach to g^*:

$$g_{\sigma_m}-g^*\approx\sigma_m^\omega+\dots\,. \tag{21.119}$$

Inserting this into the correction factor (21.114), we see that

$$C^{(n)}(p_i;\sigma_m,g^*,\mu,\mu)=1+\sigma_m^\omega\psi^{(n)}(p_i/\sigma_m;g^*,\mu,\mu)+\dots\,, \tag{21.120}$$

In the scaling limit $\sigma_m\rightarrow 0$, a finite correction to scaling is observed if $\psi^{(n)}$ is homogenous in the variables p_i/σ_m of degree ω. For the two-point vertex function:]

$$C^{(2)}(p_i;\sigma_m,g^*,1,1)\overset{m\approx 0}{\approx}1+\text{const}\times(p/\mu\sigma_m)^\omega+\dots\,. \tag{21.121}$$

Then

$$\Gamma(p;g,m,\mu)=\sigma_m^2\,\exp\left[-2\int_1^{\sigma_m}\frac{d\sigma'}{\sigma'}\gamma(g_{\sigma'})\right]\Gamma\left(p/\sigma_m,g^*,\mu,\mu\right)C^{(2)}(p;\sigma_m;g_{\sigma_m},\mu,\mu) \tag{21.122}$$

behaves for $t\approx 0$ like

$$\Gamma(p;g,m,\mu)\quad\overset{m\approx 0}{\approx}\quad p^{2-\eta}f(p/\mu t^\nu)\left[1+(g-g^*)\times\text{const}\times\left(\frac{p}{\mu}\right)^\omega+\dots\right]. \tag{21.123}$$

Thus the approach to scaling is controlled the exponent ω, the slope of the beta function at the fixed point g^*.

From the above discussion it is obvious that for an infrared stable fixed point, ω is positive.

At this point one may wonder about the universality of this result since, in principle, other corrections to scaling might arise if higher powers of the field were included in the energy functional, for example ϕ^6 or $\phi^2(\partial\phi)^2$. Those terms are found to be irrelevant by dimensional considerations and by studying the renormalization group equations in the presence of such terms. The scaling behavior and the approach to it remain unchanged.

21.8 Explicit Solution of the RGE close to D=4 Dimensions

Up to the two-loop level, the β-function was found in (21.54) to have in $D = 4 - \epsilon$ dimensions the simple form

$$\beta(g) = -\epsilon g + bg^2 \tag{21.124}$$

with $b = (N + 8)/6$. This function starts out with negative slope and has a zero at

$$g^* = \epsilon/b. \tag{21.125}$$

If ϵ is small enough, this statement is reliable even if we know $\beta(g)$ only to order g^2 in per turbation theory. Inserting (21.124) into equation (21.63) we may calculate with $\sigma \equiv \mu_1/\mu$ and rewriting $g(\mu\sigma)$ briefly as $g(\sigma)$,

$$\log \sigma = \int_g^{g(\sigma)} \frac{dg}{-\epsilon g + bg^2}. \tag{21.126}$$

Here we realize the important consequence of the zero in the β-function: If g is sufficiently close to the zero g^* then, in the limit $\sigma \longrightarrow 0$, the value $g(\sigma)$ always runs into g^* independent on whether $g = g(1)$ lies slightly above or below g^*. The point g^* is called a *fixed point* of the renormalization group equation. Since g^* is reached in the limit $\sigma \longrightarrow 0$ one speaks of an infrared stable fixed point. The flow of $\gamma(\sigma)$ when sending $\sigma \longrightarrow 0$ is illustrated in Fig. (21.2) by an arrow. Using the variable $1/g$ instead of g, Eq. (21.126) becomes

$$\log \sigma = \frac{1}{\epsilon} \int_{1/g}^{1/g(\sigma)} \frac{dx}{1/g^* - x}. \tag{21.127}$$

This can be integrated directly to

$$\sigma = \frac{|1/g^* - 1/g(\sigma)|^{1/\epsilon}}{|1/g^* - 1/g|^{1/\epsilon}}, \tag{21.128}$$

so that

$$g(\sigma) = \frac{g^*}{1 + \sigma^\epsilon\,(g^*/g - 1)}. \tag{21.129}$$

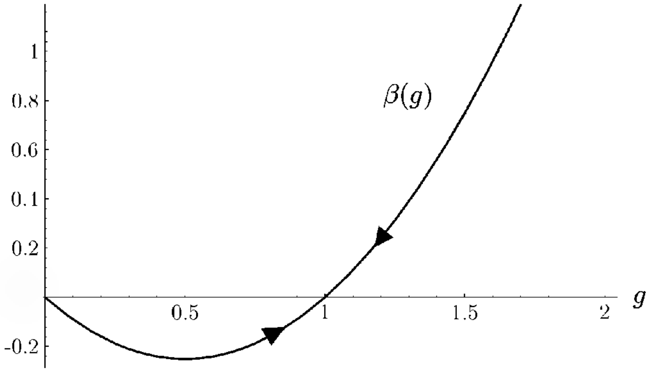

FIGURE 21.2 Flow of the coupling constant $g(\sigma)$ as the scale parameter σ approaches zero (infrared limit). For the opposite direction (ultraviolet limit), the arrows are reversed.

In general, the β-function may behave in many different ways for larger g. In particular, there may be more zeros to the right of g^*. We can see from Eq. (21.126) that for negative $\beta(g)$, the coupling constant $g(\sigma)$ will always runs towards zero from the right. The opposite statement holds for positive $\beta(g)$.

In general, the initial coupling $g(\mu) \approx g$ can flow only into the zero which lies in its *range of attraction*. In the present case this is guaranteed, for small ϵ, if g is sufficiently small.

In the limit $\sigma \longrightarrow \infty$, we see from Eq. (21.129) that g_σ tends to zero which is the other trivial zero of the beta function. This happens for any zero with a positive slope of $\beta(g)$. The limit $\sigma \longrightarrow \infty$ corresponds to $m^2 \longrightarrow \infty$, and for this reason such zeros are called *ultraviolet stable*.

In the limit $\sigma \longrightarrow \infty$, the coubling constant goes to zero, $g(\sigma) \longrightarrow 0$. In this limit $\gamma(g(\sigma)) \longrightarrow 0$ and $\gamma_m(g(\sigma)) \longrightarrow 0$. Then scaling relation (21.77) ensures $\sigma_m = m/\mu$, and the correlation functions behave like

$$\Gamma^{(n)}(p_i; g, m, \mu) \overset{m \approx 0}{\approx} \left(\frac{m}{\mu}\right)^{D-n(D/2-1)} \Gamma^{(n)}(p_i/(m/\mu); 0, \mu, \mu). \tag{21.130}$$

This is the behavior of a free-field theory where the fields fluctuate in a trivial purely Gaussian way. The zero in $\beta(g)$ at $g = 0$ is therefore called the *trivial* or *Gaussian fixed point*. In the ϕ^4-theory, the Gaussian fixed point is ultraviolet-stable (UV-stable). Since the theory tends in th limit $m \longrightarrow \infty$ against a free theory, one also says that it is ultraviolet-free. Note that this is true only in less than 4 dimensions. In $D = 4$ dimensions where $\varepsilon = 0$, the beta function has only one fixed point, the trivial Gaussian fixed point at the origin. The theory is UV unstable and IR trivial.

It is interesting to observe in which way the renormalization group equation (21.126) sums up an infinite number of diagrams of the perturbation expansion. To

At the one-loop level, the perturbative relation (21.38) between bare and renormalized coupling constant is according to (21.51) [and using $g^* = \epsilon/b$ from (21.125)]:

$$g_0 = g\mu^\epsilon \left[1 + g\frac{N+8}{9\epsilon} + \mathcal{O}(g^2)\right] = g\mu^\epsilon \left[1 + \frac{g}{g^*} + \mathcal{O}(g^2)\right]. \tag{21.131}$$

This may be rewritten as

$$\frac{1}{g_0\mu^{-\epsilon}} = \frac{1}{g} - \frac{1}{g^*} + \mathcal{O}(g). \tag{21.132}$$

The solution (21.71), on the other hand, can be brought to the form

$$\frac{1}{g_\sigma} - \frac{1}{g^*} = \sigma^\epsilon \left(\frac{1}{g} - \frac{1}{g^*}\right). \tag{21.133}$$

This solution may be compared with the perturbative one in the limit of large σ where g_σ is small. In this limit we identify

$$\frac{1}{g_0(\mu\sigma)^{-\epsilon}} = \frac{1}{g_\sigma} - \frac{1}{g^*}. \tag{21.134}$$

With this, Eq. (21.71) yields

$$\frac{1}{g_0\mu^{-\epsilon}} = \frac{1}{g} - \frac{1}{g^*}. \tag{21.135}$$

This differs from the perturbative equation (21.136) by having *no hiher order correction terms* collected in $\mathcal{O}(g)$. The renormalization group equation has resummed the first-order result (21.136) to (21.135). By taking the inverse of (21.135) we find the geometric series

$$g_0\mu^{-\epsilon} = g\left[1 + \left(\frac{g}{g^*}\right)^2 + \left(\frac{g}{g^*}\right)^3 + \mathcal{O}(g^4)\right]. \tag{21.136}$$

Since the first correction is due to a single loop, this series corresonds to summing up arbitrarily long chains of loops.

A relation of the type (21.135) was encountered before in the context of exactly solvable O(N)-symmetric ϕ^4-theories. Indeed, that relation being exact must also be an exact solution of the renormalization group equation. The difference between that and the present equation is a factor 3 which is due to the fact that for $N \to \infty$ only one of the three Wick contractions contributes [recall the discussion after Eq. (17.58)].

The power of the renormalization group is to allow us to take the perturbative equation (21.131) to the scaling limit which corresponds to replacing that equation by by

$$g_0 = g_\sigma(\sigma\mu)^\epsilon \left[1 + \frac{g_\sigma}{g^*} + \mathcal{O}(g^2)\right], \tag{21.137}$$

and letting $\sigma \to 0$ in that equation where the left-hand side becomes large and the expansion on the right-hand side is useless.

The problem appears even more dramatically by using the opposite equation

$$g_\sigma = g_0(\sigma\mu)^{-\epsilon}\left[1 - \frac{g_0(\sigma\mu)^{-\epsilon}}{g^*} + \mathcal{O}(g_0^2)\right], \tag{21.138}$$

where the terms on the right-hand side diverge increasingly fast for higher orders. The resummed form of this equation is from (21.135):

$$\frac{1}{g_\sigma} = \frac{1}{g_0(\sigma\mu)^{-\epsilon}} + \frac{1}{g^*}, \tag{21.139}$$

from which one deduces directly that $g \to g^*$ in the scaling limit $\sigma \to 0$.

The critical coupling g^* where $\beta(g)$ vanishes can be calculated for the O(N)-symmetric ϕ^4 theory in $4-\epsilon$ dimensions as a power series expansion in ϵ starting from Eq. (21.54) [recalling the reduced matrix elements T_{D_1} etc. calculated in Eqs. (9.228) (9.240)]:

$$\begin{aligned} g^* &= \frac{2}{3T_I}\epsilon + \left(\frac{3}{2}T_{I_4} - \frac{1}{12}T_{D_3}\right)\left(\frac{2}{3T_I}\right)^3 \epsilon^2 + \dots \\ &= \frac{6}{N+8}\left[\epsilon + 3\frac{3N+14}{(N+8)^2}\epsilon^2 + \dots\right]. \end{aligned} \tag{21.140}$$

Inserting this into (21.55) and (21.56) we find the ϵ expansions for $\gamma^*, \gamma^*_{m^2}$ up to this order:

$$\gamma^* \equiv \gamma(g^*) = \frac{1}{108}\frac{T_{D_3}}{T_I^2}\epsilon^2 = \frac{1}{4}\frac{N+2}{(N+8)^2}\epsilon^2 \equiv \frac{\eta}{2}, \tag{21.141}$$

$$\begin{aligned} \gamma^*_{m^2} - 2\gamma^* &\equiv \bar\gamma_{m^2}(g^*) \\ &= \frac{1}{3}\frac{T_{D_1}}{T_I}\epsilon + \left[\frac{4}{27}\left(\frac{3}{2}T_{I_4} - \frac{1}{12}T_{D_3}\right)\frac{T_{D_1}}{T_I} - \frac{1}{9}T_{D_3}\right]\frac{\epsilon^2}{T_I^2} \\ &= \frac{N+2}{N+8}\epsilon\left[1 + 6\frac{N+3}{(N+8)^2}\epsilon\right] = 2 - \nu^{-1} - \eta, \end{aligned} \tag{21.142}$$

so that

$$\gamma^*_{m^2} = \frac{N+2}{N+8}\epsilon\left[1 + \frac{13N+44}{2(N+8)^2}\epsilon\right] = 2 - \nu^{-1}. \tag{21.143}$$

The last equation yields the ϵ-expansion for the critical exponent ν:

$$\nu = \frac{1}{2} + \frac{N+2}{4(N+8)}\epsilon + \frac{(N+2)(N+3)(N+20)}{8(N+8)^3} + \dots. \tag{21.144}$$

For $\omega = d\beta/dg|_{g=g^*}$ we obtain from (21.54) and (21.140)

$$\omega = \epsilon + \left(\frac{1}{3}T_{D_3} - 6T_{I_4}\right)\left(\frac{\epsilon}{3T_I}\right)^2 = \epsilon - 3\frac{3N+14}{(N+8)^2}\epsilon^2 + \dots\ . \tag{21.145}$$

21.9 Further Critical Relations

We shall now derive some more consequences of the above general scaling relations (21.73), (21.101), (21.112). To have some specific physical system in mind, we may think of $\phi(x)$ for $N = 3$ as describing the local fluctuating magnetization in some magnetic system. fluctuating magnetization field. At the mean-field level we see that if the square mass m^2 is larger than zero, the field expectation value $\Phi = \langle\phi\rangle$ vanishes. This corresponds to being above the transition temperature for magnetic ordering. For $m^2 < 0$, on the other hand, the value Φ becomes non-zero $\pm\sqrt{6m^2/g}$. This corresponds to the spontaneous magnetization of a ferromagnet. Certainly, in a proper magnetic system, the magnetization can take any spatial directions, while in the model with a real ϕ field allows only for two opposite directions. An improvement can be made by letting Φ be a vector field and this will be done in a later section. It should, however, be noted that experimentally it is possible to find special magnetic systems in which the lattice anisotropy inhibits strongly the rotational degrees of freedom and favors only two directions of magnetization. Such systems are referred to as *Ising like*. The following discussions will apply to these if we identify Φ with the Ising like magnetization $M \equiv M_z$. A linear coupling to an external current j in the effective action

$$\Gamma[\Phi; g, m^2, \mu] + \int d^Dx\Phi j \equiv \Gamma[M, g, m^2, \mu] + \int d^DxMH \tag{21.146}$$

is then to be interpreted as coupling to an external magnetic field.

The mass square is identified with the relative temperature distance from critical value as in

From what we have learned in the Section (21.6), we may conclude that the fixed point at $g = g^*$ governs the leading behaviour of all vertex functions close to the critical point.

The critical exponents ν, η, ω determine the critical behavior of all observables and the approach to this behavior.

Let us derive the scaling relations of several important thermodynamic quantities and correlation functions.

21.9.1 Scaling Relations Above T_c

Consider at first the regime $T \geq T_c$ with a vanishing external field H.

Specific Heat Consider the specific heat as a function of temperature. The ground state energy above T_c is given by the effective potential at zero average field $v(\Phi = 0)$, which according to (21.103) and (21.79) has the scaling behavior

$$v(\Phi = 0) \overset{m\approx 0}{\approx} \sigma_m^D \times \text{const.} \approx \tau^{D/(2-\gamma_m^*)}. \tag{21.147}$$

Forming twice the derivative with respect to τ we find for the specific heat at constant volume

$$C \overset{t\approx 0}{\approx} \tau^{D/(2-\gamma_m^*)-2} = \tau^{D\nu-2}, \qquad \tau > 0. \tag{21.148}$$

This behaviour has been observed experimentally and the critical exponent has been named α:

$$C \overset{t\approx 0}{\approx} t^{-\alpha}; \qquad t > 0. \tag{21.149}$$

Thus we can identify

$$\alpha = 2 - D/(2-\gamma_m^*) = 2 - D\nu. \tag{21.150}$$

Susceptibility Suppose now that the system at $T > T_c$ is brought into an external field $j \neq 0$ which we shall call "magnetic field" settin $j = M$ (indicating applications to magnetism). The equilibrium value of the internal "magnetic field" $M \equiv Phi$ is no longer zero but $M_H \equiv \Phi_j$. It is determined by the equation of state

$$j = \left.\frac{\partial v(\Phi)}{\partial \Phi}\right|_{\Phi_j}. \tag{21.151}$$

From (21.103) we see that

$$j \overset{\tau\approx 0}{\approx} \sigma_m{}^{D-\gamma^*-(D/2-1)} v'(\Phi/\sigma_m^{\gamma^*+D/2-1}; g^*, \mu, \mu), \qquad \tau > 0. \tag{21.152}$$

The *susceptibility* is obtained by an additional differentiation

$$\chi^{-1} \equiv \left.\frac{\partial^2 v}{\partial \Phi^2}\right|_{\Phi=\Phi_j} \overset{\tau\approx 0}{\approx} \sigma_m{}^{D-(D-2)} \sigma_m^{-2\gamma^*} v''(\Phi/\sigma_m^{\gamma^*+D/2-1}; g^*, \mu, \mu), \qquad \tau > 0. \tag{21.153}$$

For $\tau > 0$ and zero field $H \equiv j$ one has $\Phi = 0$, and finds

$$\chi^{-1} \propto \sigma_m^{2-2\gamma^*} = \tau^{2(1-\gamma^*)/(2-\gamma_m^*)}. \tag{21.154}$$

Experimentally, this critical exponent is called γ:

$$\chi^{-1} \overset{\tau\approx 0}{\approx} \tau^{\gamma}, \qquad \tau > 0. \tag{21.155}$$

Hence we can identify

$$\gamma = 2\frac{1-\gamma^*}{2-\gamma^*} = \nu(2-\eta). \tag{21.156}$$

Critical Magnetization At the critical point, the proportionality of H and M is destroyed by quantum fluctuations. Experimentally one observes

$$H \to M^{\delta}; \quad t = 0. \tag{21.157}$$

Equation (21.152) shows that if the effective potential is to be finite at the critical point where $\sigma_m = 0$, the derivative v' must behave like some power

$$v' \overset{t\approx 0}{\approx} \text{const.} \times \left(\Phi/\sigma^{\gamma^*+D/2-1}\right)^{\delta}, \qquad t > 0 \tag{21.158}$$

then, since $j \propto \sigma_m^{D-\gamma^*-(D/2-1)} v'$, the power δ which makes j finite for $\sigma_m \to 0$ must satisfy

$$D - \gamma^* - (D/2-1) + [\gamma^* + (D/2-1)]\,\delta = 0. \tag{21.159}$$

From this we obtain

$$\delta = \frac{D+2-2\gamma^*}{D-2+2\gamma^*} = \frac{D+2-\eta}{D-2+\eta}. \tag{21.160}$$

21.9.2 Scaling Relations Below T_c

Let us now turn to scaling results *below* T_c. Since all individual vertex functions in the expansion of the effective action (21.89) can be calculated for $m^2 < 0$ just as well as for $m^2 > 0$, the main difference lies in $v(\Phi)$ not having a minimum at $\Phi = 0$ but at $\Phi = \Phi_0 \neq 0$ for vanishing external fields. In addition, the scaling variable σ_m is not fixed by the condition (21.72), but by a similar relation with an opposite sign

$$m_\sigma^2/\sigma^2|_{\sigma=\sigma_m} = -\mu^2, \tag{21.161}$$

so that we obtain via (21.74) the relation

$$-\frac{m^2}{\mu^2} \overset{m\approx 0}{\approx} \exp\left\{\int_0^{\sigma_m} \frac{d\sigma'}{\sigma'}\,[2-\gamma_{m^2}(g^*)]\right\} = \sigma_m^{2-\gamma^*_{m^2}}. \tag{21.162}$$

rather than (21.76), leading to

$$\sigma_m \approx (-\tau)^{1/(2-\gamma^*_{m^2})} \tag{21.163}$$

instead of (21.79).

Spontaneous Magnetization Consider first the behaviour of the spontaneous magnetization $M_0 \equiv \Phi_0$ as the temperature approaches T_c from below. The equilibrium value of Φ is determined by the minimum of the effective potential $v(\Phi)$. According to the general scaling form (21.103), the minimum must be situated at a fixed

$$\Phi_0/\sigma_m^{\gamma^*+D/2-1} = \text{const}\,. \tag{21.164}$$

Hence Φ_0 depends on m^2 and thus on the reduced temperature t as follows:

$$M_0 \equiv \Phi_0 \propto \sigma_m^{\gamma^*+D/2-1} = (-\tau)^{(\gamma^*+D/2-1)/(2-\gamma^*_m)}. \tag{21.165}$$

Thus we derive the experimentally observable relation

$$M_0 \equiv \Phi_0 \propto (-\tau)^\beta \tag{21.166}$$

with the critical exponent [not to be confused with the β-function (21.31)]

$$\beta = \frac{\gamma^* + D/2 - 1}{2-\gamma^*_m} = \frac{\nu}{2}(D-2+\eta). \tag{21.167}$$

Coherence Length Consider now the temperature dependent coherence length below T_c. From (21.112) we read off that the two-point function satisfies

$$\Gamma^{(2)}(p;\Phi_0,g,m^2,\mu)\overset{\tau\approx 0}{\approx}\sigma_m^{2-2\gamma^*}\Gamma^{(2)}\left(p/\sigma_m;\Phi_0/\sigma_m^{\gamma^*+D/2-1},g^*,\mu,\mu\right),\quad \tau>0 \tag{21.168}$$

As in the previous case $T > T_c$, this is a function of

$$p/\sigma_m=\xi(\tau)p, \tag{21.169}$$

with the same temperature behavior as in (21.87). The same critical exponent governs the divergence of the coherence lengtk below and above T_c.

This above-below symmetry is found for the critical indices α and γ of specific heat and susceptibility. When deriving the scaling behavior for $\tau < 0$, we have to keep track of the change of the abverage field Φ_0 with temperature.

Specific Heat The exponent of the specific heat, α', follows now from the potential

$$v(\Phi_0)\overset{t\approx 0}{\approx}{\sigma_m}^D v\left(\Phi_0/\sigma_m^{\gamma^*+D/2-1},g^*,\mu,\mu\right),\quad \tau>0. \tag{21.170}$$

Since the temperature change of Φ_0 takes place at a constant combination (21.164), the presence of $\Phi_0 \neq 0$ can be ignored and we obtain the same result as in (21.147), implying a temperature behaviour

$$v(\Phi_0)\propto\sigma_m^D\sim\tau^{D\nu}. \tag{21.171}$$

This agrees with the $T > T_c$ behavior (21.147), leading to the same critical exponent of the specific heat as in (21.150).

Susceptibility Suppose now that an external magnetic field is switched on. The equilibrium value Φ shifts by $\delta\Phi \equiv \Phi_j - \Phi_0$ from Φ_0 to Φ_j, which is determined by (21.151), (21.152). For $\delta\Phi$ we obtain the scaling relation

$$j\rightarrow\sigma_m^{D-(\gamma^*+D/2-1)}v'((\Phi_0+\delta\Phi)/\sigma_m^{\gamma^*+D/2-1},g^*,\mu,\mu). \tag{21.172}$$

Expanding this to first order in $\delta\Phi$ gives

$$\delta j\rightarrow\delta\Phi\,\sigma_m^{2-2\gamma^*}v''(\Phi_0/\sigma_m^{\gamma^*+D/2-1},g^*,\mu,\mu). \tag{21.173}$$

Since Φ_0 changes with t according to (21.166), the last factor is independent of temperature, and the susceptibility $\chi(t)$ has the same functional form as in (21.153), exhibiting the same critical exponent γ as in (21.155).

Widom's Relation Finally it is worth noting that Eq. (21.152) corresponds exactly to a scaling relation proposed and investigated first by Widom (1965) for the free energy at a fixed magnetization M:

$$F(t,M) = \tau^{2-\alpha}\psi(\tau/M^{1/\beta}), \tag{21.174}$$

where ψ is some smooth function of its arguments.

Differentiating this with respect to M, we find the magnetic equation of state

$$H = \tau^{2-\alpha}M^{-1-1/\beta}\psi'(\tau/M^{1/\beta}). \tag{21.175}$$

This can be rewritten as

$$\frac{H}{M^\delta} = f\left(\frac{\tau}{M^{1/\beta}}\right) \tag{21.176}$$

with some function $f(x)$, as is easily proved by inserting on the left-hand side the scaling relation $\delta = -1 + (2-\alpha)/\beta$. In terms of the variables of our field theory, the equation of state (21.176) may be rewritten as

$$j = \tau^{\delta\beta}\left(\frac{\tau}{\Phi^{1/\beta}}\right)^{-\delta\beta} f\left(\frac{\tau}{\Phi^{1/\beta}}\right) = \tau^{\delta\beta} g\left(\frac{\Phi}{\tau^\beta}\right), \tag{21.177}$$

where $g(x)$ is some other function. By comparing this with (21.152) we see that

$$\delta\beta = [D - \gamma^* - (D/2-1)]\frac{1}{2-\gamma_m*} = \frac{\nu}{2}(D+2-\eta). \tag{21.178}$$

21.10 Comparison of Scaling Relations with Experiment

For a comparison with experiment we may pick three two sets of critical data and extract the values of η, ν, and ω. The remaining critical indices can then be found from the above-derived scaling relations which we summarized, for convenience:

$$\alpha = \alpha' = 2 - 2\beta - \gamma, \tag{21.179}$$

$$\gamma = \gamma' = \nu(2-\eta) \tag{21.180}$$

$$\gamma = \nu(2-\eta), \tag{21.181}$$

$$\nu D = 2 - \alpha. \tag{21.182}$$

$$\delta = \frac{D+2-\eta}{D-2+\eta}. \tag{21.183}$$

As an example take the magnetic system $CrBr_3$ where one measures

$$\beta \approx 0.368, \quad \delta \approx 4.3, \quad \gamma \approx 1.215.$$

Inserting these into the scaling relation

$$\beta = \gamma/(\delta - 1) \tag{21.184}$$

which folows (21.179) and (21.183), we see that it is satisfied excellently. Inserting δ into the relation

$$\eta = \frac{D+2-(D-2)\delta}{\delta+1} \tag{21.185}$$

we find for $D = 3$

$$\eta \approx 0.132, \tag{21.186}$$

and from the relation $\nu = \gamma(2-\eta)$,

$$\nu \approx 0.65. \tag{21.187}$$

Results from ϵ-Expansion

Let us compare these numbers with the results from the ϵ expansion. Using Eqs. (21.140) - (21.142) and the above formulas for the critical indices in terms of γ^*, $\gamma_{m^2}*$ we find the series for the two independent critical indices.

$$\eta = \frac{N+2}{2(N+8)^2}\epsilon^2 + \dots \tag{21.188}$$

$$\nu = \frac{1}{2} + \frac{N+2}{4(N+8)}\epsilon + \frac{(N+2)(N^2+23N+60)}{8(N+8)^3}\epsilon^2 + \dots\ . \tag{21.189}$$

These results are valid only for infinitesimal ϵ. For applications, one assumes that the ϵ expansions can be used also in $D = 3$ dimensions, i.e. for $\epsilon = 1$, where physics takes place. The justification of this rather ad hoc procedure lies in an approximate numerical decrease of the ϵ and ϵ^2 terms in (21.140,21.142). Thus we find for $N = 1, 2, \infty$,

$$\begin{aligned} \nu &= \tfrac{1}{2} + \tfrac{1}{12}\epsilon + \tfrac{7}{9\cdot 9\cdot 2}\epsilon^2 + \dots = \tfrac{203}{9\cdot 9\cdot 4} + \dots \approx 0.627, && N = 1,\\ \nu &= \tfrac{1}{2} + \tfrac{1}{10}\epsilon + \tfrac{11}{200}\epsilon^2 + \dots = \tfrac{131}{200} + \dots \approx 0.655, && N = 2,\\ \nu &= \tfrac{1}{2} + \tfrac{1}{4}\epsilon + \tfrac{1}{8}\epsilon^2 + \dots = \tfrac{7}{8} + \dots \approx 0.875, && N = \infty. \end{aligned} \tag{21.190}$$

The other critical index is

$$\begin{aligned} \eta &= \tfrac{1}{54}, && N = 1,\\ \eta &= \tfrac{1}{15}, && N = 2,\\ \eta &= \tfrac{1}{2}, && N = \infty, \end{aligned} \tag{21.191}$$

in the three cases.

The ϵ-expansion for ν has decreasing contributions of the higher orders. The value up to order ϵ^2, $\nu \approx 0.627$, is in reasonable agreement with the experimantal value $\nu \approx 0.65$. $\nu^{-1} - 2 = -\frac{1}{3}, \nu \sim 0.6$ and this is in good agreement with the experimental value (21.187) here from p.30.

There is only one term to order ϵ so no convergence can be judges. The agreement with experiment reasonable. The value to order ϵ^2 at $\epsilon = 1$ is $\eta \approx 0.019$ which, via the scaling relation $\nu = \gamma/(2-\eta)$, corresponds to $\nu \approx 0.61$, quite close to the experimental value 0.65.

It is not advisable to calculate to higher order than ϵ^2 since the agreement to order ϵ^3 usually becomes worse. In fact, the series does not converge and it is meaningless to carry the expansion any further. The rough agreement up to order ϵ is a consequence of the *asymptotic convergence* of the series. the

21.11 Higher-Order Expansion

Let us state the presently known higher powers in ϵ up to order ϵ^4 one finds[1] after much work the beta function

$$
\begin{aligned}
\beta(g) \;=\; & \tfrac{g^2}{6}[N+8] \;-\; \tfrac{g^3}{6}[3N+14] \\
& +\tfrac{g^4}{432}\;[33N^2+922N+2960\;+\;\zeta(3)\cdot 96(5N+22)] \\
& -\tfrac{g^5}{7776}\;[-5N^3+6320N^2+80456N+196648 \\
& \qquad +\zeta(3)\cdot 96(63N^2+764N+2332) \\
& \qquad -\zeta(4)\cdot 288(5N+22)(N+8) \\
& \qquad +\zeta(5)\cdot 1920(2N^2+55N+186)] \\
& +\tfrac{g^6}{124416}[13N^4+12578N^3+808496N^2+6646336N+13177344 \\
& \qquad +\zeta(3)\cdot 16(-9N^4+1248N^3+67640N^2+552280N+1314336) \\
& \qquad +\zeta^2(3)\cdot 768(-6N^3-59N^2+446N+3264) \\
& \qquad -\zeta(4)\cdot 288(63N^3+1388N^2+9532N+21120) \\
& \qquad +\zeta(5)\cdot 256(305N^3+7466N^2+66986N+165084) \\
& \qquad -\zeta(6)(N+8)\cdot 9600(2N^2+55N+186) \\
& \qquad +\zeta(7)\cdot 112896(14N^2+189N+526)]\;,
\end{aligned}
\tag{21.192}
$$

and the critical indices

$$
\begin{aligned}
\eta(\varepsilon) \;=\; & \tfrac{(N+2)\varepsilon^2}{2(N+8)^2}\Big\{1+\tfrac{\varepsilon}{4(N+8)^2}[-N^2+56N+272] \\
& -\tfrac{\varepsilon^2}{16(N+8)^4}[5N^4+230N^3-1124N^2-17920N-46144 \\
& \qquad +\zeta(3)(N+8)\cdot 384(5N+22)] \\
& -\tfrac{\varepsilon^3}{64(N+8)^6}[13N^6+946N^5+27620N^4+121472N^3 \\
& \qquad -262528N^2-2912768N-5655552 \\
& \qquad -\zeta(3)(N+8)\cdot 16(N^5+10N^4+1220N^3-1136N^2-68672N-171264) \\
& \qquad +\zeta(4)(N+8)^3\cdot 1152(5N+22) \\
& \qquad -\zeta(5)(N+8)^2\cdot 5120(2N^2+55N+186)]\Big\}\;,
\end{aligned}
\tag{21.193}
$$

---

[1] See H. Kleinert, J. Neu, V. Schulte-Frohlinde, K.G. Chetyrkin, and S.A. Larin, Phys. Lett. B *272*, 39 (1991).

and

$$
\begin{aligned}
1/\nu(\varepsilon) \;=\; & 2+\tfrac{(N+2)\varepsilon}{N+8}\Big\{-1-\tfrac{\varepsilon}{2(N+8)^2}(13N+44) \\
& +\tfrac{\varepsilon^2}{8(N+8)^4}\,[3N^3-452N^2-2672N-5312 \\
& \qquad +\zeta(3)(N+8)\cdot 96(5N+22)] \\
& +\tfrac{\varepsilon^3}{32(N+8)^6}\,[3N^5+398N^4-12900N^3-81552N^2-219968N-357120 \\
& \qquad +\zeta(3)(N+8)\cdot 16(3N^4-194N^3+148N^2+9472N+19488) \\
& \qquad +\zeta(4)(N+8)^3\cdot 288(5N+22) \\
& \qquad -\zeta(5)(N+8)^2\cdot 1280(2N^2+55N+186)] \\
& +\tfrac{\varepsilon^4}{128(N+8)^8}[3N^7-1198N^6-27484N^5-1055344N^4 \\
& \qquad -5242112N^3-5256704N^2+6999040N-626688 \\
& \qquad -\zeta(3)(N+8)\cdot 16(13N^6-310N^5+19004N^4+102400N^3 \\
& \qquad\qquad -381536N^2-2792576N-4240640) \\
& \qquad -\zeta^2(3)(N+8)^2\cdot 1024(2N^4+18N^3+981N^2+6994N+11688) \\
& \qquad +\zeta(4)(N+8)^3\cdot 48(3N^4-194N^3+148N^2+9472N+19488) \\
& \qquad +\zeta(5)(N+8)^2\cdot 256(155N^4+3026N^3+989N^2-66018N-130608) \\
& \qquad -\zeta(6)(N+8)^4\cdot 6400(2N^2+55N+186) \\
& \qquad +\zeta(7)(N+8)^3\cdot 56448(14N^2+189N+526)]\Big\}\,,
\end{aligned}
\tag{21.194}
$$

The higher orders in ϵ start growing rapidly for $\epsilon = 1$ after the ϵ^0, ϵ^1 terms there is no convergence. In fact, it can easily be shown that the series is only an asymptotic expansion. Resummation techniques are needed to extract reliable informations.[2]

21.12 Mean-Field Results for Critical Indices

In mean-field theory fluctuations are neglected and the effective action is equal to the bare action with the quantum field ϕ replaced by the expectation value $\Phi = \langle\phi\rangle$:

$$
\Gamma[\Phi] = \int d^Dx \left[\frac{1}{2}(\partial\Phi)^2 - \frac{m^2}{2}\Phi^2 - \frac{g}{4}\Phi^4 + \Phi j\right]. \tag{21.195}
$$

The mass is assumed to behave as

$$
m^2 = \mu^2\left(\frac{T}{T_c}-1\right) \equiv \mu^2\tau, \tag{21.196}
$$

and Φ and j are interpreted as magnetization M and field H, respectively. The two-point function is

$$
\Gamma^{(2)}(p) = p^2 - m^2, \tag{21.197}
$$

---

[2] For a detailed discussion and the many references see the textbook W. Janke and H. Kleinert, *Borel Resummation of Divergent Perturbation Series*, World Scientific Publ. Comp., Singapore, 1997. This book contains many references to the original papers.

from which we read off, at $m^2 = 0$ or $T = T_c$, that the critical index η which determines the power behaviour of the correlation function vanishes:

$$\eta = 0. \tag{21.198}$$

Above T_c, we rewrite $\Gamma^{(2)}$ in the rescaled form (21.70):

$$\Gamma^{(2)}(p; g, m, \mu) = \sigma^2 \left[(p/\sigma)^2 - m^2/\sigma^2\right]. \tag{21.199}$$

Thus we identify $\sigma_m = m/\mu$ and the coherence length has the temperature behaviour

$$\xi(\tau) = \frac{1}{\mu\sigma_m} = \frac{1}{m} \sim \tau^{-1/2}. \tag{21.200}$$

This implies the critical index

$$\nu = \frac{1}{2}. \tag{21.201}$$

We now turn to the regime $T < T_c$. Then the effective potential has a nontrivial minimum at

$$\Phi_0 = \sqrt{-\frac{m^2}{g}} \propto (-\tau)^{1/2}. \tag{21.202}$$

The critical exponent β is therefore determined to be

$$\beta = \frac{1}{2}. \tag{21.203}$$

Inserting $\Phi = \Phi_0 + \delta\Phi$ into the effective action (21.195), we find the two-point function below T_c

$$\Gamma^{(2)} = \left.\frac{\delta^2\Gamma}{\delta\Phi\delta\Phi}\right|_{\Phi=\Phi_0} = p^2 + 2m^2. \tag{21.204}$$

This shows that the coherence length is equal to

$$\xi(\tau) = \frac{1}{\sqrt{-2m^2}} \sim \tau^{-1/2}. \tag{21.205}$$

Hence the index ν' below T_c is the same as ν above T_c:

$$\nu' = \frac{1}{2}. \tag{21.206}$$

Consider now the specific heat. The equilibrium energy above T_c and below T is:

$$\begin{aligned} \nu &\equiv 0, & T &\geq T_c, \\ \nu &\equiv -\frac{m^4}{4g}, & T &< T_c, \end{aligned} \tag{21.207}$$

respectively. Differentiating this twice with respect to m^2 we see that

$$C = \text{const}\,, \quad T < T_c, \tag{21.208}$$

which implies that

$$\alpha' = 0. \tag{21.209}$$

Note that the index α above T_c is undetermined at the mean-field level since $C \equiv 0$.

Let us now allow for a nonzero magnetic field. Then for $T < T_c$, the equilibrium value of Φ_0 i given by

$$m^2\Phi_0 + g\Phi_0^3 = j. \tag{21.210}$$

For $T = T_c$, this has the solution

$$j = g\Phi_0^3 \tag{21.211}$$

so that we can read off [see (21.157)]

$$\delta = 3. \tag{21.212}$$

For $T > T_c$, we see that for small j

$$\Phi \approx \frac{1}{m^2}j \tag{21.213}$$

so that the susceptibility is

$$\chi \approx (m^2)^{-1} \propto \tau^{-1}, \tag{21.214}$$

giving the critical index [see (21.155)]

$$\gamma = -1. \tag{21.215}$$

Below T_c, on the other hand, we insert $\Phi = \Phi_0 + \delta\Phi$ and find

$$(m^2 + 3g\Phi_0^2)\delta\Phi = j \tag{21.216}$$

or

$$\delta\Phi = -\frac{1}{2m^2}j \tag{21.217}$$

which amounts to

$$\chi = -\frac{1}{2m^2} \propto (-\tau)^{-1}. \tag{21.218}$$

Thus γ' is the same as γ:

$$\gamma' = \gamma = -1. \tag{21.219}$$

Note that χ measures the size of the fluctuations of the magnetization field $M(\mathbf{x})$ around the equilibrium value. It is determined by the curvature of the effective potential at the minimum. Above T_c this is m^2, below T_c it is twice the opposite of m^2 (which is again positive).

The critical indices satisfy the general scaling relations (21.179) (21.183). Indeed, with $\nu = \eta/2 = 0$, wee see that the relations are

$$\alpha = \alpha' = 2 - \frac{D}{2}, \quad \delta = \frac{D+2}{D-2}, \quad \gamma = \gamma' = 1, \quad \beta = \frac{1}{2}\left(\frac{D}{2} - 1\right). \tag{21.220}$$

For $D = 4$ they yield once more the above derived mean field exponent.

21.13 Effective Potential in the Critical Regime to Order ϵ

From (21.103), (21.77), (21.86), and (21.167), the effective potential has for small mass values the universal form

$$\begin{aligned} v(\Phi; g, m, \mu) &\xrightarrow{m\to 0} \mu^D \left(\frac{m^2}{\mu^2}\right)^{D\nu} w\left(\frac{\Phi/\mu^{(D-2)/2}}{(m^2/\mu^2)^{\nu(\gamma^*+D/2-1)}}\right) \\ &= \mu^D \tau^{D\nu} w\left(\frac{\Phi/\mu^{(D-2)/2}}{\tau^\beta}\right), \end{aligned} \tag{21.221}$$

where w is some dimensionless function. In the presence of an external magnetic field $H \equiv j$, this corresponds to an equation of state in the Widom form (21.177):

$$j = \frac{\partial v}{\partial \Phi} = \mu^{D/2+1} \tau^{D\nu-\beta} w'\left(\frac{\Phi/\mu^{(D-2)/2}}{\tau^\beta}\right) = \tau^{\delta\beta} g\left(\frac{\Phi}{\tau^\beta}\right). \tag{21.222}$$

We shall now demonstrate how the function w can be calculated at the one-loop level. The renormalization group analysis of the previous sections made statements only on the numerical values for the critical indices. Nothing was known on the specific shape of the effective action v and thus of the general Widom function $f(x)$. To lowest order in ϵ it is possible to calculate v from the one-loop effective potential.

Consider the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{m^2}{2}\phi^2 - \frac{g_0}{4}\mu^\epsilon \phi^4. \tag{21.223}$$

We have taken the factor μ^ϵ out of g_0 to make it g_0 a dimensionless number in $D = 4 - \epsilon$ dimensions. The one-loop correction to the effective action is calculated in the usual way. The partition function reads

$$Z = \int \mathcal{D}\phi e^{i\mathcal{A}[\phi]/\hbar} = \int \mathcal{D}\phi e^{(i/\hbar)\int d^D x \mathcal{L}(x)}. \tag{21.224}$$

Expanding around the classical solution

$$\phi(x) = \Phi + \delta\phi(x), \tag{21.225}$$

the exponent has the lowest terms

$$\int d^D x \mathcal{L}(\Phi) - \int d^D x \frac{1}{2}\delta\phi(x)\left(\partial^2 + m_0^2 + \frac{g_0}{2}\mu^\epsilon\Phi^2\right)\delta\phi(x) + \dots\ . \tag{21.226}$$

Performing the path integral over the quadratic fluctuations gives

$$\begin{aligned} Z &\approx e^{(i/\hbar)\int d^D x \mathcal{L}(\Phi)} \det{}^{-1/2}\left(\partial^2 + m_0^2 + \frac{g_0}{2}\mu^2\Phi^2\right) \\ &= \exp\left\{\frac{i}{\hbar}\left[\int d^D x \mathcal{L}(\Phi) + \frac{i}{2}\hbar\, \mathrm{Tr}\log\left(\partial^2 + m_0^2 + \frac{g_0}{2}\mu^\epsilon\Phi^2\right)\right]\right\} \equiv e^{i\mathcal{A}_{1\,\text{loop}}[\Phi]}. \end{aligned} \tag{21.227}$$

As was shown before one can replace Φ directly by the extremal value in the one-loop corrected action $\mathcal{A}_{1\,\mathrm{loop}}[\Phi]$, thus obtaining the correct effective action $\Gamma[\Phi]$ to order $\hbar$. The evaluation is easiest at a constant Φ field where $\Gamma[\Phi]$ determines the effective potential as

$$v(\Phi) = -L^D \Gamma[\Phi]|_{\Phi=const},$$

with L^D being the volume of the system in D dimensions. Then the trace of the logarithm is simply the integral

$$\sum_{\mathbf{p}} \log\left(-p^2 + m_0^2 + \frac{g_0}{2}\mu^\epsilon \Phi^2\right) = L^D \int \frac{d^D p}{(2\pi)^D} \log\left(-p^2 + m_0^2 + \frac{g_0}{\epsilon}\mu^\epsilon \Phi^2\right),$$

and the effective potential at the one-loop level reads

$$v(\Phi) = \frac{m_0^2}{2}\Phi^2 + \frac{g_0}{4!}\mu^\epsilon \Phi^4 - \frac{i}{2}\hbar \int \frac{d^D p}{(2\pi)^D} \log\left(-p^2 + m^2 + \frac{g_0}{\epsilon}\mu^\epsilon \Phi^2\right). \tag{21.228}$$

Performing a Wick rotation to euclidean momenta p_ϵ^μ with $p_E^2 = -p^2$, $d^D p \equiv i d^D p_E$, the third term becomes

$$\frac{1}{2}\int \frac{d^D p_E}{(2\pi)^D} \log\left(p_E^2 + m_0^2 + \frac{g_0}{2}\mu^\epsilon \Phi^2\right). \tag{21.229}$$

This integral was calculated in Eq. (9.133) for all dimensions D as

$$\int \frac{d^D p_E}{(2\pi)^D} \log(p_E^2 + m_0^2) = \bar{S}_D \frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}(m_0^2)^{D/2}. \tag{21.230}$$

This brings the the potential to the form

$$v = \frac{m^2}{2}\Phi^4 + \frac{g}{4!}\mu^\epsilon \Phi^4 + \frac{1}{2}\bar{S}_D \frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}(m_0 + \frac{g_0}{2}\mu^\epsilon \Phi^2)^{D/2}. \tag{21.231}$$

It will be more convenient to consider directly the equation of state rather than v itself and derive

$$j = \frac{\partial v}{\partial \Phi} = m_0^2 \Phi + \frac{g_0}{3!}\mu^\epsilon \Phi^3 + \frac{1}{4}\bar{S}_D \Gamma(2-\epsilon/2)\Gamma(-1+\epsilon/2)\hbar g_0 \mu^\epsilon \Phi \left(m_0^2 + \frac{g_0 \mu^\epsilon}{2}\Phi^2\right)^{1-\epsilon/2}. \tag{21.232}$$

Close to $\epsilon = 0$, the last term can be expanded as

$$-\frac{g_0 \mu^\epsilon}{2}\bar{S}\Phi\left(\frac{1}{\epsilon} + \mathcal{O}(\epsilon)\right)\left(m_0^2 + \frac{g_0 \mu^\epsilon}{2}\Phi^2\right)\mu^{-\epsilon}\left[1 - \frac{\epsilon}{2}\log\left(\frac{m_0^2}{\mu^2} + \frac{g_0 \mu^\epsilon}{2}\frac{\Phi^2}{\mu^2}\right) + \mathcal{O}(\epsilon)\right]. \tag{21.233}$$

According to the minimal substraction scheme in dimensional regularization we may simply drop the singular $1/\epsilon$-piece and arrive at the renormalized expression

$$j = \frac{\partial v}{\partial \Phi} = m^2\Phi + \frac{g}{3}\mu^\epsilon\Phi^3 + \hbar\frac{S_D g}{4}(m^2 + \frac{g}{2}\mu^\epsilon\Phi^2)\Phi\log\left(\frac{m^2}{\mu^2} + \frac{g}{2}\mu^\epsilon\frac{\Phi^2}{\mu^2}\right). \quad (21.234)$$

The potential is

$$v = \frac{m^2}{2}\Phi^2 + \frac{g\mu^\epsilon}{3!}\Phi^3 + \hbar\frac{S}{8}\mu^{-\epsilon}\left(m^2 + \frac{g\mu^\epsilon}{2}\Phi^2\right)^2\left[\log\left(\frac{m^2}{\mu^2} + \frac{g}{2}\mu^\epsilon\frac{\Phi^2}{\mu^2}\right) - \frac{1}{2}\right]. \quad (21.235)$$

Let us now see how these expressions can be brought to the universal forms (21.221), (21.222). Neglecting, for a moment, the logarithmic $\hbar$-correction, we rewrite the first two terms in (21.234) as

$$\begin{aligned} j = \frac{\partial v}{\partial \Phi} &= \mu^{3+\epsilon/2}\frac{\Phi}{\mu^{1+\epsilon/2}}\left(\frac{m^2}{\mu^2}\right)\left[1 + \frac{g}{3!}\left(\frac{\Phi}{\mu^{1+\epsilon/2}}\Big/\sqrt{\frac{m^2}{\mu^2}}\right)^2\right] \\ &= \mu^{3+\epsilon/2}\left(\frac{m^2}{\mu^2}\right)^{3/2}\left(\frac{\Phi}{\mu^{1+\epsilon/2}}\Big/\sqrt{\frac{m^2}{\mu^2}}\right)\left[1 + \frac{g}{3!}\left(\frac{\Phi}{\mu^{1+\epsilon/2}}\Big/\sqrt{\frac{m^2}{\mu^2}}\right)^2\right] \end{aligned} \quad (21.236)$$

Comparing this with (21.222), we can identify the mean-field critical indices [as in (21.203), (21.212)]

$$\delta = 3, \quad \beta = \frac{1}{2}. \quad (21.237)$$

We shall now calculate the lowest-order corrections to thse critical indices by considering two specific scaling relations. First, we consider the limit $\Phi \to 0$. Since for $\tau > 0$, the derivative $\partial v/\partial\Phi$ has to carry a factor Φ, equation (21.222) shows that $\partial v/\partial\Phi$ should behave as a function of τ as follows

$$j \propto \Phi\mu^2\tau^{D\nu - 2\beta} = \Phi\mu^2\tau^{(\delta-1)\beta} = \Phi\mu^2\tau^\gamma. \quad (21.238)$$

From (21.236) we see, on the other hand, that

$$j = \frac{\partial v}{\partial \Phi} = \Phi\mu^2\frac{m^2}{\mu^2}\left(1 + \hbar\frac{S_D g}{4}\log\frac{m^2}{\mu^2}\right). \quad (21.239)$$

This is a first-order expansion in g of the power law

$$= \Phi\mu^2\left(\frac{m^2}{\mu^2}\right)^{1+\hbar S_D g/4} + \mathcal{O}(g^2). \quad (21.240)$$

From this, we read off the one-loop corrected critical exponent which rules the divergence of the magnetic susceptibility near the critical point via $\xi \propto \tau^{-\gamma}$:

$$\gamma \equiv \nu(2-\eta) = 1 + \frac{\hbar S_D g}{4} + \mathcal{O}(g^2). \quad (21.241)$$

For a second independent exponent we work directly at the critical point $m = 0$. By Widom's relation, $\partial v/\partial\Phi$ behaves like $\left(\Phi/\mu^{(D-2)/2}\right)^{\delta}$. From (21.236) we find the power law

$$\begin{aligned}
\frac{\partial v}{\partial \Phi} &= \frac{g}{3!}\mu^{3-\frac{5}{2}\epsilon}\sqrt{\frac{2}{g}}^{3}\left(\sqrt{\frac{g}{2}}\frac{\Phi}{\mu^{1-\epsilon/2}}\right)^{3}\left[1+\hbar\frac{\bar{S}_D g}{2}\log\left(\sqrt{\frac{g}{2}}\frac{\Phi}{\mu^{1-\epsilon}}\right)\right]\\
&= \frac{g}{3!}\mu^{3-\frac{5}{2}\epsilon}\left(\frac{2}{g}\right)^{3/2}\left(\sqrt{\frac{g}{2}}\frac{\Phi}{\mu^{1-\epsilon/2}}\right)^{3+\hbar 3\,\bar{S}_D g/2} + \mathcal{O}(g^2). \qquad (21.242)
\end{aligned}$$

We can therefore identify the critical index δ with which the critical magnetization responds to an external field (in the scaling law $H \propto M^{\delta}$)

$$\delta = 3 + \hbar\frac{3}{2}\bar{S}_D g + \mathcal{O}(g^2). \qquad (21.243)$$

Using (21.179) (21.183) we can calculate the exponent

$$\beta = \frac{D\nu}{1+\delta} \qquad (21.244)$$

which rules the way in which the spontaneous magnetization vanishes for $\tau \to -0$ [in the scaling law $M \propto (-\tau)^{\beta}$]. Further

$$\nu = \frac{\gamma}{D}\frac{\delta+1}{\delta-1} \qquad (21.245)$$

governing the divergence of the coherence length (in $\xi \propto \tau^{-\nu}$). Note that β satisfies the scaling relation

$$\beta = \frac{\gamma}{\delta - 1}, \qquad (21.246)$$

as it should according to (21.184). Inserting (21.241) and (21.243) we find

$$\beta = (1+\hbar\bar{S}g/4)/(2+\hbar\frac{3}{2}\bar{S}_D g) = \frac{1}{2} - \hbar\bar{S}g/4 + \mathcal{O}(g^2). \qquad (21.247)$$

We can use these results to explicitly find the function $g(x)$ in the universal Widom expressions (21.222), (21.177) at the one-loop level. We define the dimensionless field variable

$$y = \sqrt{\frac{g}{2}}\frac{\Phi}{\mu^{1-\epsilon/2}} \qquad (21.248)$$

and the combined variable occuring in (21.242)

$$x \equiv \tau/y^{1/\beta}. \qquad (21.249)$$

Then $\partial v/\partial\Phi$ in (21.242) is expressible in the form

$$\frac{\partial v}{\partial \Phi} = \Phi\,\mu^{2} y^{\delta-1} f(x), \qquad (21.250)$$

with a function $f(x)$ related to the potential v by

$$f\left(\sqrt{\frac{2}{g}}x\right) = x^{-\delta} v'(x). \tag{21.251}$$

By rewriting (21.236) in terms of y we find

$$\frac{\partial v}{\partial \Phi} = \Phi\, \mu^2 \left[(\tau + y^2/3) + \hbar \frac{S_D g}{4}(\tau + y^2)\log(\tau + y^2)\right]. \tag{21.252}$$

Upon identifying

$$x = \frac{\tau}{y^{1/\beta}} = \frac{\tau}{y^{2+\hbar\, S_D g}} \approx \frac{\tau}{y^2}\left(1 - \hbar S \frac{g}{2}\log y^2\right), \tag{21.253}$$

this can obviously be brought to the form

$$\begin{aligned}\frac{\partial v}{\partial \Phi} = \Phi\, \mu^2 y^{\delta - 1}\left(1 - \hbar S \frac{3}{4} g \log y^2\right)\left\{\left[\frac{1}{3} + x\left(1 + \hbar S \frac{g}{2}\log y^2\right)\right]\right. \\ \left. + \hbar S g/4\left[(1+x)\left(1 + \hbar S \frac{g}{2}\log y^2\right)\right] \times \left[\log y^2 + \log(1+x)\left(1 + \hbar S \frac{g}{2}\log y^2\right)\right]\right\}.\end{aligned} \tag{21.254}$$

Since we are working at the one-loop level, the g^2 corrections can be neglected and we remain with

$$\frac{\partial v}{\partial \Phi} = \Phi\, \mu^2 y^{\delta - 1}\left[\left(\frac{1}{3} + x\right) + \hbar \frac{S_D g}{4}(1+x)\log(1+x)\right]. \tag{21.255}$$

To the same order in g, this is the same as

$$\frac{\partial v}{\partial \Phi} = \Phi\, \mu^2 y^{\delta - 1}\left[-\frac{2}{3} + (1+x)^{\gamma}\right]. \tag{21.256}$$

We have identified the leading power of $1 + x$ with γ since it determines the τ-behaviour of the susceptibility for $\Phi \to 0,\ x \to \infty$. The expression (21.256) is of the desired universal form (21.250).

Note that at the one-loop level, this form has been obtained by working purely in 4 dimensions and calculating the correction to order g. Nowhere have we needed the ϵ-expansion and the critical indices δ, γ etc. as functions of the running coupling constant $g(\mu)$. Continuation to $4 - \epsilon$ dimensions bcomes only necessary as we are trying to approach the physical situation $D = 3$. If we move only an infinitesimal piece ϵ away from $D = 4$, the running coupling stabilizes at $\hbar S_D g = \frac{2}{3}\epsilon$. This is extracted from the coupling constant renormalization

$$\frac{1}{g(\mu)} = \frac{\mu^{\epsilon}}{g_0} - \frac{3 S_D \hbar}{2\epsilon} \tag{21.257}$$

by going to the infrared limit $\mu \to 0$. This is what finally determines the critical indices as functions of ϵ:

$$\begin{aligned}\delta &= 3+\epsilon, \qquad \eta=0,\\ \beta &= \frac{1}{2}-\frac{\epsilon}{6}, \quad \gamma = 1+\epsilon/6,\\ \nu &= \frac{1}{2}+\frac{\epsilon}{12}.\end{aligned} \tag{21.258}$$

If the function $f(x)$ in the universal form (21.250) is desired to higher orders in ϵ, the calculation becomes quite cumbersome already at the next order in ϵ.

21.14 O(N)-Symmetric Theory

For completeness, let us generalize the previous calculation to the full O(N)-symmetric case with the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial\phi_a)^2 - \frac{m_0^2}{2}\phi_0^2 - \frac{g_0}{4!}\mu^\epsilon(\phi_a^2)^2. \tag{21.259}$$

Now the quadratic fluctuations are given by

$$\delta^2\mathcal{A} = \int d^4x\frac{1}{2}\delta\phi_a\left[-\partial^2 - m_0^2 - \frac{g_0\mu^\epsilon}{6}(\delta_{ab}\Phi^2+2\Phi_a\Phi_b)\right]\delta\phi_b \tag{21.260}$$

so that the one-loop corrected effective action becomes

$$\begin{aligned}\Gamma[\Phi] = \frac{1}{2}(\partial\Phi_a)^2 - \frac{m_0^2}{2}\Phi_a^2 - \frac{g_0\mu^\epsilon}{4}(\Phi_a^2)^2\\ -\frac{i}{2}\hbar\mathrm{tr}\log\left[(-\partial^2-m^2)\delta_{ab} - \frac{g_0\mu^\epsilon}{6}(\delta_{ab}\Phi^2+2\Phi_a\Phi_b)\right],\end{aligned} \tag{21.261}$$

with an effective potential

$$v[\Phi] = \frac{m_0^2}{2}\Phi_a^2 + \frac{g_0\mu^\epsilon}{4!}(\Phi_a^2)^2 + \frac{1}{2}\mathrm{tr}\int\frac{d^Dp_E}{(2\pi)^D}\log\left[(p_E^2+m^2)\delta_{ab}+\frac{g_0\mu^\epsilon}{6}(\delta_{ab}\Phi^2+2\Phi_a\Phi_b)\right]. \tag{21.262}$$

The trace of the logarithm of the matrix calculated as the sum of the logarithms of the eigenvalues which are, obviously,

$$p^2 + m_0^2 + \frac{g_0\mu^\epsilon}{6N}\Phi^2 \tag{21.263}$$

for the $N-1$ unit vectors orthogonal to Φ and

$$p^2 + m^2 + \frac{g_0\mu^\epsilon}{2N}\Phi^2 \tag{21.264}$$

for the Nth unit vector parallel to Φ_a: Hence

$$v(\Phi) = \frac{m_0^2}{2}\Phi_a^2 + \frac{g_0\mu^\epsilon}{4!N}(\Phi_a)^2 \tag{21.265}$$
$$+\frac{\hbar}{2}\int\frac{d^Dp_E}{(2\pi)}\left[(N+1)\log\left(p_E^2+m_0^2+\frac{g_0\mu^\epsilon}{6N}\Phi^2\right)+\log(p_E^2+m_0^2+\frac{g_0\mu^2}{2N}\Phi^2)\right].$$

Performing the momentum integral, this becomes

$$v(\Phi_a) = \frac{m_0^2}{2}\Phi_a^2 + \frac{g_0\mu^\epsilon}{4!N}(\Phi_a^2)^2 + \frac{\hbar}{2}\bar{S}\frac{1}{2}\Gamma(D/2)\Gamma(1-D/2)\frac{2}{D}$$
$$\times\left[(N-1)(m_0^2+\frac{g_0\mu^\epsilon}{6N}\Phi^2))^{D/2}+(m_0^2+\frac{g_0\mu^\epsilon}{2\omega}\Phi^2)^{D/2}\right]. \tag{21.266}$$

The corresponding equation is

$$j_a = \frac{\partial v(\Phi_a)}{\partial\Phi_a} = \Phi_a\left\{m_0^2+\frac{g_0\mu^\epsilon}{3!}\Phi_a^2+\hbar\frac{g_0\mu^\epsilon}{4N}\bar{S}\Gamma(D/2)\Gamma(1-D/2)\right.$$
$$\left.\times\left[\frac{1}{3}(N-1)(m_0^2+\frac{g_0\mu^\epsilon}{6N}\Phi^2)+(m_0^2+\frac{g_0\mu^\epsilon}{2N}\Phi^2)^{1-\epsilon/2}\right]\right\}. \tag{21.267}$$

Expanding this to lowest order in $\epsilon = 4-D$, we find after renormalization

$$v(\Phi) \;=\; \frac{m^2}{2}\Phi_a^2+\frac{g\mu^\epsilon}{4!}(\Phi_a^2)^2+\hbar\mu^{-\epsilon}\frac{\bar{S}}{8}\left\{(N-1)(m^2+\frac{g\mu^\epsilon}{6}\Phi^2)^2\log(m^2+\frac{g\mu^\epsilon}{6}\Phi^2)\right.$$
$$\left.+(m^2+\frac{g}{2}\Phi^2)^2\log(m^2+\frac{g\mu^\epsilon}{2}\Phi^2)\right\}. \tag{21.268}$$

with an equation of state

$$j_a = \frac{\partial v}{\partial\Phi_a} = \Phi_a\left\{m^2+\frac{g\mu^\epsilon}{3!}\Phi_a^2+\hbar\frac{g}{4}\bar{S}\left[\frac{1}{3}(N-1)(m^2+\frac{g\mu^\epsilon}{6}\Phi_a^2)\log(m^2+\frac{g\mu^\epsilon}{6}\Phi_a^2)\right.\right.$$
$$\left.\left.+(m_0^2+\frac{g\mu^\epsilon}{2}\Phi_a^2)\log(m^2+\frac{g\mu^\epsilon}{2}\Phi_a^2)\right]\right\}. \tag{21.269}$$

Again we may identify the susceptibility by taking $\Phi_a \to 0$

$$j_a = m^2\left\{1+\hbar\frac{g\mu^\epsilon}{4D}\left[\frac{1}{3}(N-1)+1\right]\log m^2\right\} \approx (m^2)^{1+\hbar\frac{g\mu^\epsilon}{4}\bar{S}\frac{N+2}{3}+\mathcal{O}(g^2)} \tag{21.270}$$

so that [compare (21.241)]

$$\gamma = 1+\hbar\frac{g\mu^\epsilon}{4}\bar{S}_D\frac{N+2}{3}. \tag{21.271}$$

The index δ is found by comparing the $m^2 = 0$ -relation (21.250) [recall also (21.242)]

$$j_a \to \Phi_a\frac{g\mu^\epsilon}{3!}\Phi_a^2\left[1+\left(\frac{N-1}{3}+3\right)\hbar\frac{g\mu^\epsilon}{4}\log\Phi^2\right] \tag{21.272}$$

with the defining relation

$$j_a \approx \Phi_a \left(\Phi_a^2\right)^{(\delta-1)/2}. \tag{21.273}$$

This gives

$$\frac{\delta-1}{2} = 1 + \hbar\frac{S_D g\mu^\epsilon}{4}\left(\frac{N-1}{3}+3\right). \tag{21.274}$$

Using the same reduced variables as before, i.e.,

$$\begin{aligned} y &= \sqrt{\frac{g}{2}}\frac{\sqrt{\Phi_a^2}}{\mu^{1-\epsilon/2}} \\ x &= \tau/y^{1/\beta}, \quad m^2 = \mu^2\tau, \end{aligned} \tag{21.275}$$

the equation of state can be brought to the universal form

$$\begin{aligned} j_a = \frac{\partial v}{\partial \Phi_a} = \Phi_a\mu^2 y^{\delta-1}\Bigg\{\left(\frac{1}{3}+x\right) \\ +\hbar S\frac{g}{4}\left[\frac{1}{3}(N-1)\left(1+\frac{x}{3}\right)\log\left(1+\frac{x}{3}\right)+(1+x)\log(1+x)\right]\Bigg\}. \end{aligned} \tag{21.276}$$

Using again γ, this can be rewritten, in analogy with (21.256), as

$$j_a = \frac{\partial v}{\partial \Phi_a} = \Phi_a\mu^2 y^{\delta-1}\left\{\frac{2}{3}(N-2)+\frac{3}{N+2}(1+x)^\gamma+\frac{N-1}{N+2}\left(1+\frac{x}{3}\right)^\gamma\right\}. \tag{21.277}$$

At this level, the indices δ and γ do not yet have their infrared fixed point values. From (21.140) we know that the fixed-point lies at

$$g^* \equiv \hbar g S = \frac{6\epsilon}{N+8}. \tag{21.278}$$

This allows us to express δ in terms of ϵ as

$$\delta = 3+\epsilon, \tag{21.279}$$

valid for any N. Actually, this would have followed directly from the general scaling relations (21.179) (21.183) and the fact that the anomalous dimension η vanishes to order ϵ [see (21.141).

Finally, comparing (21.271) with (21.278) we obtain

$$\gamma = 1+\frac{1}{2}\frac{N+2}{N+8}\epsilon. \tag{21.280}$$

Thus we can calculate the other critical indices as

$$\nu = \frac{\gamma}{2-\eta} = \frac{1}{2}+\frac{N+2}{4(N+8)}\epsilon, \tag{21.281}$$

$$\beta = \gamma(\delta-1) = \frac{1}{2}-\frac{3}{2(N+8)}\epsilon. \tag{21.282}$$

21.15 Direct Scaling Form in the Limit of Large N

In the limit $N \to \infty$, effective action and potential are known exactly and it is possible to retrieve the scaling properties most directly. Consider the potential in $D = 4 - \epsilon$ dimensions as calculated in (8.4): (here we use $\frac{g_0}{N}$ as a coupling constant rather than g_0)

$$v(\Phi) = \frac{1}{2}\Delta\,\Phi_a^2 + \frac{m_0^2}{2g_0} - \frac{N}{4g_0}\Delta^2 + \frac{1}{2}NS\frac{1}{2}\Gamma(2-\epsilon/2)\Gamma(-1+\epsilon/2)\frac{2}{4-\epsilon}\Delta^{2-\epsilon/2}, \tag{21.283}$$

where Δ is the function of Φ_a^2:

$$\Phi_a^2 = \frac{N}{g_0}\Delta - \frac{Nm_0^2}{g_0} - NS\frac{1}{2}\Gamma(2-\epsilon/2)\Gamma(-1+\epsilon/2)\Delta^{1-\epsilon/2}. \tag{21.284}$$

We see that m_0^2 and Φ_a^2 scale in the same way so that v is a function of Φ_a^2/m_0^2 and m_0^2. If we let $m_0^2 \to 0$ with Φ_a^2/m_0^2 fixed, the last term in Eq. (21.284) dominates the first and we find the limit

$$\left(\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0}\right) m_0^2 \xrightarrow{m_0 \to 0} -NS\frac{1}{2}\Gamma(2-\epsilon/2)\Gamma(-1+\epsilon/2)\Delta^{1-\epsilon/2}. \tag{21.285}$$

Similarly, in v the last term dominates the third so that we can write

$$\begin{aligned} v(\Phi) &\to \Delta\frac{m_0^2}{2}\left[\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0}\right] + \frac{1}{2}NS\frac{1}{2}\Gamma(2-\epsilon/2)\Gamma(-1+\epsilon/2)\frac{2}{4-\epsilon}\Delta^{2-\epsilon/2} \\ &\to \Delta\frac{m_0^2}{2}\left(\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0}\right)\frac{2-\epsilon}{4-\epsilon} \to \text{const} \times \left[m_0^2\left(\frac{\Phi_a^2}{m_0^2} + \frac{N}{g_0}\right)\right]^{1+1/(1-\epsilon/2)}. \end{aligned} \tag{21.286}$$

Comparing this with Widom's parametrization

$$v(\Phi) \sim (\Phi_a^2)^{(\delta+1)/2} f\left(\frac{m_0^2}{(\Phi_a^2)^{1/\beta}}\right), \tag{21.287}$$

we see that

$$\beta = \frac{1}{2}, \tag{21.288}$$

and

$$\frac{\delta+1}{2} = \frac{2-\epsilon/2}{1-\epsilon/2}, \tag{21.289}$$

or

$$\delta = \frac{6-\epsilon}{2-\epsilon} = \frac{D+2}{D-2}. \tag{21.290}$$

This agrees with the $N \to \infty$ limit of (21.279) (21.282).

Note that we have done the calculations in terms of the unrenormalized quantities m_0^2 and g_0. If we go over to the renormalized ones m and g, the changes affect only the terms which were dropped in the limit $m_0^2 \to 0$ [i.e. the third term in (21.280) and the first one in (21.281)]. The result remains therefore the same.

22

Internal Symmetries of Strong Interactions

If we open up a standard table of the presently known elementary particles, we see a confusing variety of many different objects. Before trying to develop a more detailed theory of their interactions it is useful to find certain organizing principles which correlate their quantum numbers and mass spectra.

22.1 Classification of Elementary Particles

The most fundamental distinction concerns the statistics of the particles which can be of the Fermi-Dirac or Bose-Einstein type in which case the particles are called fermions or bosons, respectively. Historically, the fermions were subdivided into light and heavy fermions. The former are called leptons and comprise particles such as electrons, muons, and neutrinos. Recently, also heavier objects have been found which should be considered as leptons, due to the similarity of their interactions with that of the other leptons. In fact, the characteristic property of leptons is now that they are fermions with no strong interactions. The distinction according to mass is no longer significant.
The most important of the traditional heavy fermions are the particles which make up the atomic nucleus, the so-called nucleons which can be protons and neutrons. These particles have strong interactions. They can be excited in nuclear collisions producing short-lived resonances which are also classified as elementary heavy fermions. The set of all heavy fermions with strong interactions are called baryons. All baryons can be produced in collision or decay processes also as in the form of antiparticles. These look very similar to the corresponding particles, they have exactly the same mass and spin, but other quantum numbers such as the charge are reversed.

The particles with Bose-Einstein statistics are separated into those with don't and those which do possess strong interactions. The former play an important role in the theoretical description of the gravitational, the electromagnetic, and the weak interactions. They are called graviton, photon, and intermediate vector bosons W and Z. The bosons with strong interactions are called mesons. The set of all particles with strong interactions, baryons and mesons, are called *hadrons*.

Only few of all these particles are completely stable. The most prominent ones make up the stable matter of the universe. These are the protons, electrons, photons, neutrinos, and gravitons. The proton is the only stable baryon. The other important nuclear constituent, the neutron, lives on the average only 898 ± 16 seconds. After this it decays into a proton, an electron, and an antineutrino.
Among the leptons, only electrons and neutrinos are stable particles. The muon, a particle which is very similar to the electron but much heavier, decays in about 10^{-6} seconds into an electron, a neutrino, and an antineutrino.

The proton is not only the only stable heavy fermion, it is the only stable strongly interacting particle. The mesons are all unstable.

The decays proceeding over a "long" time as in the case of the neutron are called weak. Even lifetimes of 10^{-13} seconds are still considered as long in elementary particle physics and the decay is called weak. A particle with such a lifetimes down to 10^{-11} sec leaves an observable trace in a bubble chamber.

Most of the hadrons which decay via strong interaction processes live only for a much shorter time than that, so short that they do travel any visible distance in a bubble chamber. They are observable only as resonances in scattering cross sections. The most prominent example is the first resonance in pion nucleon scattering shown in Fig. 22.2. The resonance is called $\Delta(1232)$. It lies at a pion beam momentum

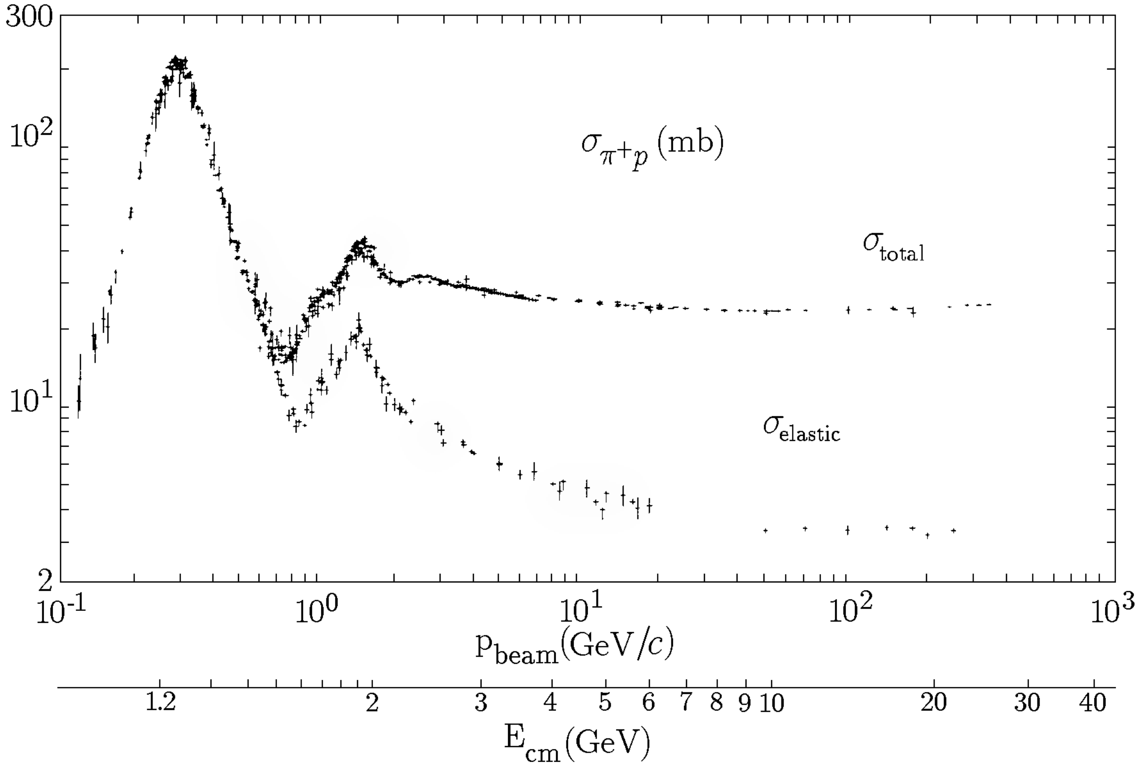

FIGURE 22.1 The total and elastic π^+ -proton cross section showing clearly the first nucleon resonance called $\Delta(1232)$.

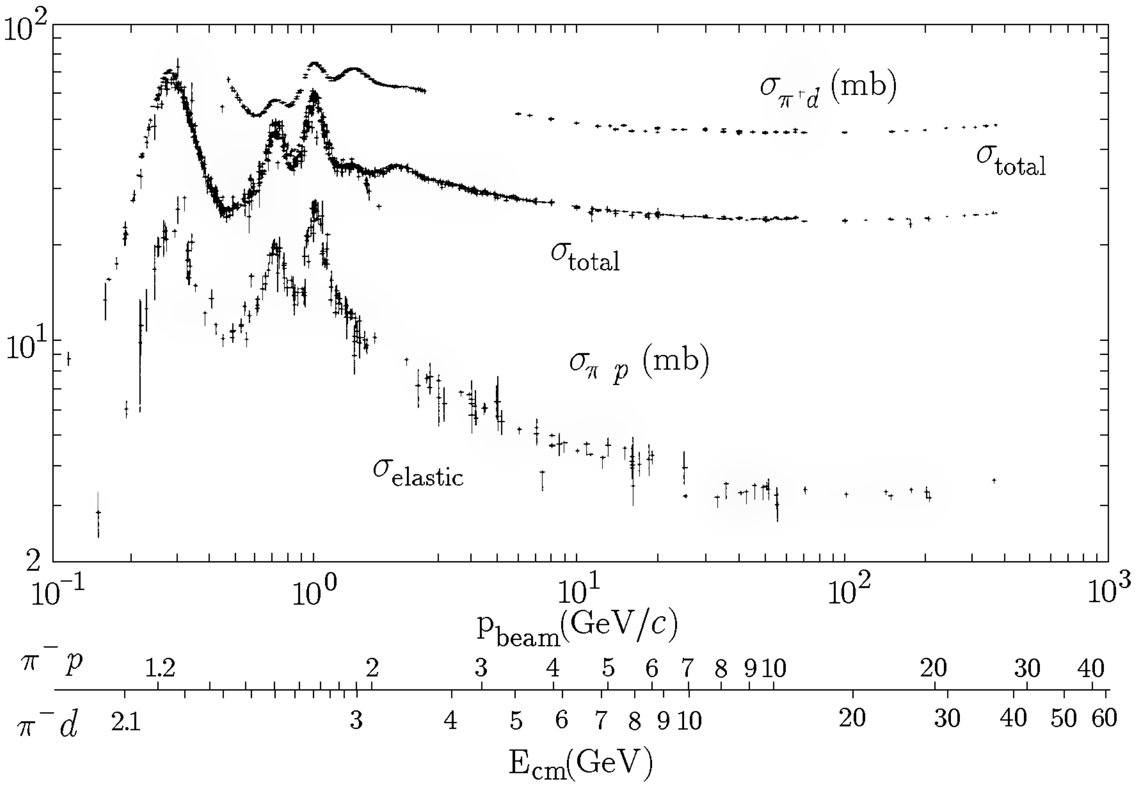

FIGURE 22.2 The total and elastic π^- -proton cross section showing again clearly the first nucleon resonance called $\Delta(1232)$, but with only a third of the height. This is in agreement with the isospin 3/2 assignment and the amplitude relations (22.39) if one invokes the optical theorem, according to which the total cross section is proportional to the imaginary part of the forward scattering amplitude.

$$p_\pi = 0.34\,\text{GeV/c}. \tag{22.1}$$

In the center of mass coordinate frame, the energy is equal to the mass of the resonance M,

$$E_{\text{CM}} = M = \sqrt{(E_\pi + m_p)^2 - p_\pi^2} = \sqrt{m_\pi^2 + m_p^2 + 2m_pE_\pi} \tag{22.2}$$

where $E_\pi = \sqrt{p_\pi^2 + m_\pi^2}$ is beam energy and m_π, m_p are the masses of pion and proton. From $p_\pi = 0.34\,\text{GeV/c}$ one finds $M = 1232\,\text{MeV/c}^2$ which is the number given in the parenthesis of $\Delta(1232)$. The large width in the total cross section shows the rather short lifetime. The peak is of the Lorentz shape and can be parametrized as

$$\sigma_{\text{tot}} \propto \frac{\Gamma}{(E_{\text{CM}} - M)^2 + (\Gamma/2)^2}. \tag{22.3}$$

At the energies $E_{\rm CM} = M \pm \Gamma/2$ the cross section has fallen to half its peak value. The parameter Γ is therefore identified with the *width* of the resonance. From the experimental curve we extract the width

$$\Gamma \approx 115 \text{ MeV}. \tag{22.4}$$

In the quantum mechanical theory of resonance scattering it is known that such a cross section indicates an exponentially decaying wave function of the form

$$\Psi \propto e^{-i(M-i\Gamma/2)t/\hbar}. \tag{22.5}$$

Indeed, such a wave function leads to a scattering amplitude which contains a pole in the energy plane below the real axis, proportional to

$$\frac{1}{E_{\rm CM} - M + i\Gamma/2}. \tag{22.6}$$

Its absolute square gives the above Lorentzian cross section. The lifetime of such a wave function is

$$\tau = 2\hbar/\Gamma. \tag{22.7}$$

This is why the inverse width is sometimes called the half-life. In physical units, the right-hand side is to be multiplied with $\hbar$ if Γ is measured in MeV and τ in seconds. The $\Delta(1231)$ resonance has therefore a lifetime

$$\begin{aligned} \tau = 2\hbar/\Gamma &= 0.6583 \times 10^{-21}\, \frac{\text{MeV}}{\Gamma}\text{sec} \\ &\approx\; 5.72 \times 10^{-24} \text{ sec}. \end{aligned} \tag{22.8}$$

It decays mostly into a pion and a nucleon. Such a short lived decay is called strong decay. A small fraction, however, about 0.6% of the decays goes into a nucleon and a photon. This is called the *radiative decay* channel.

Since the $\Delta(1232)$ resonance can decay into a nucleon and a photon, we should expect that it can also be produced in a collision of the final states, i.e., when a photon hits a nucleon. Indeed, the cross sections in Fig. 22.3 show clearly this resonance.

In the past twenty years, various simple organizing principles have been found according to which the variety of particles and resonances can be classified and remembered and their interactions be related. These principles are based on symmetry groups associated with certain characteristic invariances of the different interactions. They have helped in understanding the quantum numbers, the energy spectra, the various decay channels, and the different scattering cross sections.

22.2 Isospin in Nuclear Physics

If one compares binding energies of so-called mirror nuclei (which are obtained from each other by the interchange of protons and neutrons) with each other one

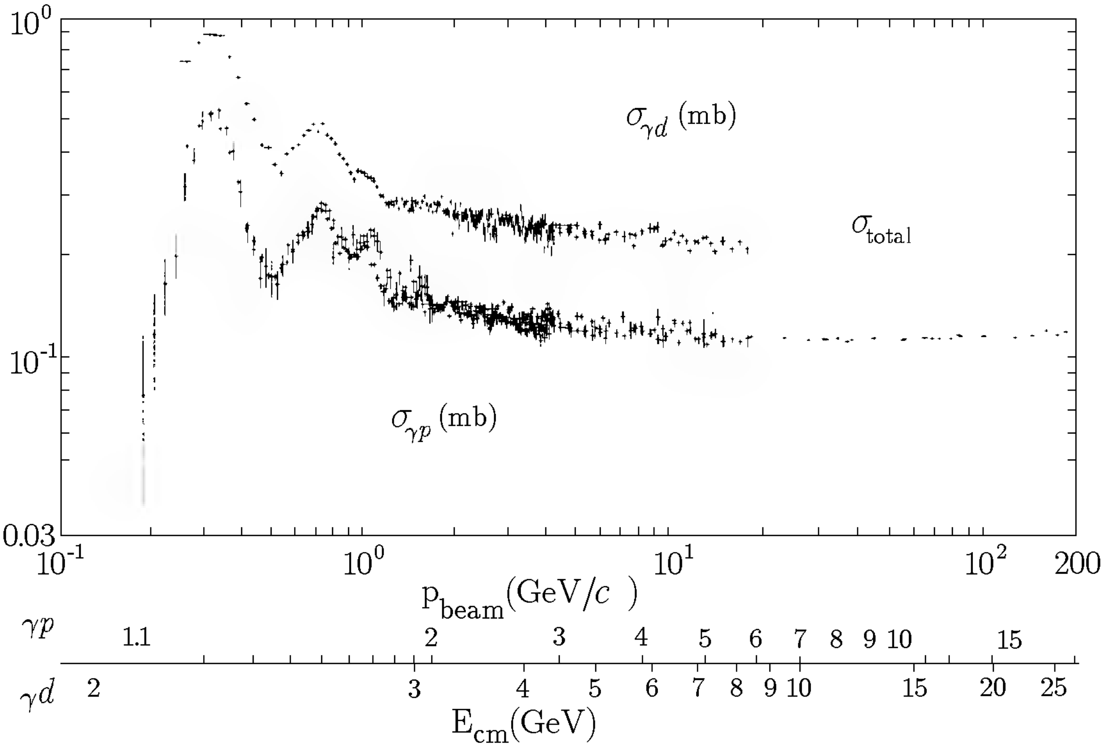

FIGURE 22.3 The photon-proton and photon-deuteron total cross sections showing clearly the first nucleon resonance $\Delta(1232)$ as well as a second resonance called $N(1520)$.

finds that the difference may be attributed entirely to the different electromagnetic interactions of protons and neutrons. For instance, $^3\text{H}= nnp$ and $^3\text{He}= ppn$ have binding energies $\text{B}_{\text{H}^3} = 8.452\,\text{MeV}$ and $\text{B}_{^3\text{He}} = 7.728\,\text{MeV}$, respectively, with the difference being accounted for by the proton-neutron mass difference $m_n - m_p = 1.293323\pm.000016\,\text{MeV}$ and by the different Coulomb field energy around the nuclei. Indeed, if the Coulomb energy is approximated by that of a uniformly charged sphere of charge Z and radius R, the field energy is

$$E_{\text{Coul}} = (1/2)(Z-1)\frac{6}{5}\frac{e^2}{4\pi R} = (1/2)Z(Z-1)\frac{6}{5}\frac{\alpha\hbar c}{R}. \tag{22.9}$$

With $\alpha = e^2/4\pi\hbar c \approx 1/137$ being the fine-structure constant. Using for the nuclear radius for the atomic number A the estimate $R \approx 1.45\,A^{1/3}\times 10^{-13}\,\text{cm}$, we can write

$$E_{\text{Coul}} \approx Z(Z-1)\frac{6}{5}\cdot A^{-1/3}\ \text{MeV}. \tag{22.10}$$

For $A = 3, Z = 2$ we estimate $E_{\text{Coul}} \approx 0.57\,\text{MeV}$ and find for the difference in binding energy

$$\text{B}_{\text{H}^3} - \text{B}_{\text{He}^3} \approx 1.29\,\text{MeV} - 0.57\,\text{MeV} \approx 0.72\,\text{MeV}, \tag{22.11}$$

in rough agreement with the observed 0.76 MeV.

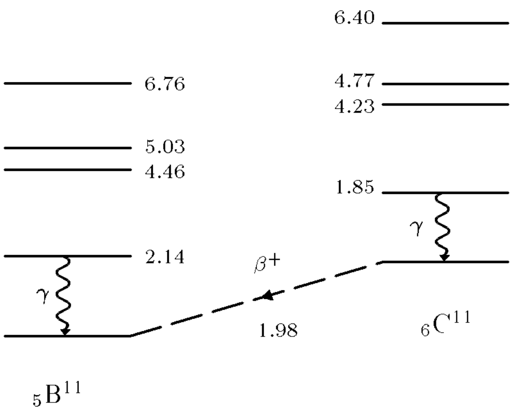

FIGURE 22.4 Mirror nuclei $_5\mathrm{B}^{11}$ and $_6\mathrm{C}^{11}$ with their excited states (the numbers are the excitation energies in MeV). The ground state of $_6\mathrm{C}^{11}$ decays into that of $_5\mathrm{B}^{11}$ by positive β-decay (i.e., emission of a positron and a neutrino) as indicated by the arrow. An estimate of the Coulomb energy via formula (22.9) explains roughly the energy difference of 1.98 between the two level schemes.

Not only the binding energies, also the excitation spectra of mirror nuclei differ only by common electromagnetic shift, as seen in the example in Fig. 22.4. This property of mirror nuclei has led nuclear theorists to postulate that if it were possible to switch off the electromagnetic interactions the potentials V_{pp} and V_{pn} would turn out to be exactly equal. This symmetry is called *c*harge symmetry.

The charge symmetry possesses a natural extension. When analyzing the data of nucleon-nucleon scattering at low energy, it was found that also also $V_{pp} \approx V_{pn}$. This led Heisenberg to postulate that within purely nuclear interactions, protons and neutrons should be two indistinguishable states of the same particle, the nucleon N. He described the two states in analogy with the two spin states of a spin 1/2 object by a two-component object

$$N = \begin{pmatrix} p \\ n \end{pmatrix}, \tag{22.12}$$

and called this object an *isospinor* state. Heisenberg considered the states as a representation of a rotation group in a fictitious space, the space of *isotopic spin*. The generators are denoted by I_i and obey the commutation rules of the rotation group

$$[I_i, I_j] = i\epsilon_{abc} I_k. \tag{22.13}$$

The two component isospinors are rotated by the 2×2 representation of I_i, given by $I_i = \sigma^i/2$. Proton and neutron are eigenstates of the third component $I_3 = \sigma^3/2$ with eigenvalue $1/2$ and $-1/2$.

The exchange of protons and neutrons corresponds to a rotation around the 2 axes of isospin by 180^0

$$e^{i\pi I_2}\begin{pmatrix} p \\ n \end{pmatrix} = e^{i\pi\sigma^2/2}\begin{pmatrix} p \\ n \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} p \\ n \end{pmatrix} = \begin{pmatrix} n \\ -p \end{pmatrix}. \tag{22.14}$$

The postulate of indistinguishability of protons and neutrons can then be formulated mathematically as the commutativity of the generators of isospin I_i with the Hamiltonian of strong interactions

$$\left[I_i, H_{\text{strong}}\right] = 0. \tag{22.15}$$

This is called *isotopic spin symmetry* or *isospin invariance* of strong interactions. If $|A\rangle$ is a nuclear n body wave function, then the isospin acts additively on each nucleon just as ordinary angular momentum (compare Appendix 3B)

$$I_i|A\rangle = (I_i \times 1 \times \ldots \times 1 + \ldots + 1 \times 1 \times 1 \times \ldots \times I_i)|A\rangle. \tag{22.16}$$

Nuclei which possess a large difference in their number of protons, n_p, and neutrons, n_n, have a third component of isospin

$$I_3|A\rangle = \frac{1}{2}(n_p - n_n)|A\rangle. \tag{22.17}$$

Their total isospin I must be at least equal to I_3. The ground state has $I = I_3$, the excited states have a higher I. If the Coulomb energies are taken into account, they can be seen to be members of isospin multiplets formed together with neighboring nuclei of equal total number of nucleons and different $n_p - n_n$ (see Fig. 22.5). With the help of isospin rotations, the charge symmetry operation may be represented as a rotation around the second axis by an angle π: $\exp(i\pi I_2)$.

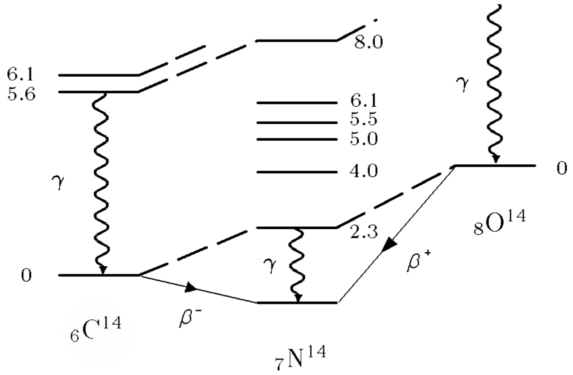

FIGURE 22.5 Singlets and triplets of isospin in the nuclei ${}_6\mathrm{C}^{14}, {}_7\mathrm{N}^{14}, {}_8\mathrm{O}^{14}$ (with the excitation energies in MeV). The dotted lines connect levels are roughly degenerate after subtracting the Coulomb energy according to the estimate (22.9).

The postulate of isopsin symmetry leads immediately to interesting selection rules for decay process via nuclear interactions, such as α decay or emission of deuterons. Consider a nucleus $|A\rangle$ that it has an equal number of protons and neutrons, i.e. a nucleus that is charge symmetric to itself, a so-called *self-conjugate nucleus*. Since it consist of an even number of isospin 1/2 nucleons, its total isopin is necessarily integer, and the third component of the isopsin is zero. The operation $\exp(i\pi I_2)$ must therefore produce the same state up to a phase η:

$$\exp(i\pi I_2)|A\rangle = \eta|A\rangle. \tag{22.18}$$

Aplying this operation twice must lead back to the original state. Hence the phase η can only be ±1. It is called the intrinsic *charge parity* of the nucleus. Every charge-symmetric nucleus has a definite charge parity.

The charge parity η is calculable uniquely as a function of the total isospin. We use the property of the eigenfunctions of angular momentum $Y_{lm}(\Theta, \varphi)$ with $m = 0$ to pick up a phase $(-)^l$, when rotated around the y-axis by an angle π [see the matrix elements of the rotation matrix (4.337)]. This is also obvious from the representation $[(I+I_3)!(I-I_3)!]^{1/2} a_p^{\dagger(I+I_3)} a_n^{\dagger(I-I_3)}|0\rangle$ of an isospin I, I_3 state in terms of creation operators $a_p^\dagger, a_n^\dagger$ of isospin up and down, as constructed in Eq. (4.322). Under an isospin rotation around the 2-axis by π, then $a_p^\dagger$ and $a_n^\dagger$ go over into $a_n^\dagger$ and $-a_p^\dagger$, respectively. A charge symmetric state with $I_3 = 0$ has therefore the charge parity

$$\eta = (-)^I. \tag{22.19}$$

The charge parity gives rise to interesting section rules for decay processes via nuclear interactions. If the Hamiltonian commutes with all generators of isospin, the initial and final states must have equal charge parities. Typical forbidden processes are

$${}_5\mathrm{B}^{*10} \begin{array}{l} \nearrow \; {}_3\mathrm{Li}^6 + \alpha \\ \searrow \; {}_4\mathrm{Be}^8 + \alpha \end{array} \tag{22.20}$$

where ${}_5\mathrm{B}^{*10}$ can be the 4.5 MeV or the 6.5 MeV resonance of ${}_5\mathrm{B}^{10}$. Now, the excited nucleus ${}_5\mathrm{B}^{*10}$ of excitation energy 4.5 MeV has is a member an $I = 1$ isospin triplet formed together with ground states of the isotopes ${}_4\mathrm{Be}^{10}$ and ${}_6\mathrm{C}^{10}$. It therefore has a charge parity $\eta = -1$. The nuclei ${}_3\mathrm{Li}^6$ and ${}_4\mathrm{Be}^8$, on the other hand, have isospin 0 and therefore a positive charge parity $\eta = +1$. They are hence forbidden processes, which have indeed never been observed in the laboratory.

Let us now study the consequences of the larger isotopic spin symmetry in nuclear reaction. A deuteron in the ground state has the orbit in a symmetric $s-$wave and the spin states are given by the three symmetric triplet states

$$|\uparrow\downarrow\rangle, \quad \frac{1}{\sqrt{2}}|\uparrow\downarrow + \downarrow\uparrow\rangle, \quad |\downarrow\downarrow\rangle.$$

The antisymmetry of the wave function requires the isotopic wave function to be antisymmetric, i.e. it must be

$$\frac{1}{\sqrt{2}}|pn - np\rangle.$$

This is an $I = 0$ state of isospin.

If a deuteron collides with ${}_4\mathrm{Be}^9$, which has $I = \frac{1}{2}, I_3 = -\frac{1}{2}$, the isospin of the two-particle system is necessarily $I = \frac{1}{2}, I_3 = -\frac{1}{2}$. We can now compare two possible final states

$$ {}_5\mathrm{B}^{*10}_{1.7\,\mathrm{MeV}} + n $$

and

$$ {}_4\mathrm{Be}^{10} + p. $$

If we denote the isospins of the two particles by $I^{(1)}, I^{(2)}$, the isospin states are in the first case

$$ |I^{(1)}, I^{(1)}_3; I^{(2)}, I^{(2)}_3\rangle = |1, 0; \tfrac{1}{2}, -\tfrac{1}{2}\rangle, \tag{22.21} $$

and in the second

$$ |I^{(1)}, I^{(1)}_3; I^{(2)}, I^{(2)}_3\rangle = |1, -1; 1, \tfrac{1}{2}\rangle. \tag{22.22} $$

The strength with which these two final states are coupled to the initial state $|\frac{1}{2}, -\frac{1}{2}\rangle$ are proportional to the Clebsch-Gordan coefficients

$$ \langle \tfrac{1}{2}, -\tfrac{1}{2}|1, 0; \tfrac{1}{2}, -\tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}}, \tag{22.23} $$

$$ \langle \tfrac{1}{2}, -\tfrac{1}{2}|1, -1; 1, \tfrac{1}{2}\rangle = \sqrt{\frac{2}{3}}, \tag{22.24} $$

respectively (recall Table 3.2). Hence the first reaction cross section should be half as big as the second, a fact born out by experiments.

22.3 Isospin in Pion Physics

In 1935 Yukawa[1] postulated the existence of a bose particle which should mediate the strong interactions between nucleons in a similar way as the photons do between atoms. From the size of nuclei being of the order of 10^{13}cm Yukawa concluded that instead of a Coulomb potential

$$ v(\mathbf{x}) = \frac{1}{4\pi r} \tag{22.25} $$

which solves the field equation

$$ -\partial_{\mathbf{x}}{}^2 v(\mathbf{x}) = \delta^{(3)}(\mathbf{x}). \tag{22.26} $$

The potential between nucleons should have a finite range and read

$$ v^Y(\mathbf{x}) = \frac{e^{-\mu r}}{4\pi r}, \tag{22.27} $$

thus solving the differential equation

$$ (-\partial_{\mathbf{x}}{}^2 + \mu^2) v^Y(\mathbf{x}) = \delta^{(3)}(\mathbf{x}). \tag{22.28} $$

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[1] H. Yukawa, Proc. Phys. Math. Soc., Japan *17*, 48 (1935).

He identified the inverse range μ with the mass of the particle. This particle was discovered experimentally around 1946 and is now called the *pion*. It exists in three charge states π^+, π^0, π^-. The neutral pion has a mass

$$m_{\pi^0} \;=\; 134.9642 \pm .0038 \text{ MeV}, \tag{22.29}$$

from which the masses of the charged pions differ by

$$m_{\pi^\pm} - m_{\pi_0} \;=\; 4.6043 \pm .00037 \text{ MeV}. \tag{22.30}$$

The π-mesons exist only for a small time. The neutral π^0 meson decays mainly into two photons with a lifetime

$$\tau_{\pi^0} \approx (0.87 \pm .04) \times 10^{-16}\text{sec}. \tag{22.31}$$

This relatively fast decay is caused purely by electromagnetic interactions. The charged $\pi^\pm$ states decay mainly into μ, ν_μ with a lifetime of

$$\tau_{\pi^\pm} \approx (2.6030 \pm 0.0023) \times 10^{-8}\text{sec}. \tag{22.32}$$

This decay is so slow that it proceeds via weak interactions.

Since nuclear forces are supposed to arise mainly from pion interactions, the isosymmetry of nuclear forces implies that the pion-nucleon coupling should be symmetric under isospin rotations. The pion itself is obviously an isospin 1 object. If it interacts with a nucleon of isospin 1/2, the total isospin can be either $\frac{3}{2}$ or $\frac{1}{2}$. The Clebsch-Gordan coefficients for the different channels of total isospin $|I, I_3\rangle$ are the following (see Table 3.2)

$$\begin{aligned}
|\pi^+p\rangle &= |1,1;\tfrac{1}{2},\tfrac{1}{2}\rangle &&= |\tfrac{3}{2},\tfrac{3}{2}\rangle,\\
|\pi^+n\rangle &= |1,1;\tfrac{1}{2},-\tfrac{1}{2}\rangle &&= \tfrac{1}{\sqrt{3}}|\tfrac{3}{2},\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}|\tfrac{1}{2},\tfrac{1}{2}\rangle,\\
|\pi^0p\rangle &= |1,0;\tfrac{1}{2},\tfrac{1}{2}\rangle &&= \sqrt{\tfrac{2}{3}}|\tfrac{3}{2},\tfrac{1}{2}\rangle - \tfrac{1}{\sqrt{3}}|\tfrac{1}{2},\tfrac{1}{2}\rangle,\\
|\pi^0n\rangle &= |1,0;\tfrac{1}{2},-\tfrac{1}{2}\rangle &&= \sqrt{\tfrac{2}{3}}|\tfrac{3}{2},-\tfrac{1}{2}\rangle + \tfrac{1}{\sqrt{3}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle,\\
|\pi^-p\rangle &= |1,-1;\tfrac{1}{2},\tfrac{1}{2}\rangle &&= \tfrac{1}{\sqrt{3}}|\tfrac{3}{2},-\tfrac{1}{2}\rangle - \sqrt{\tfrac{2}{3}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle,\\
|\pi^-n\rangle &= |1,-1;\tfrac{1}{2},-\tfrac{1}{2}\rangle &&= |\tfrac{3}{2},-\tfrac{3}{2}\rangle.
\end{aligned}$$

From these we find the amplitudes for scattering processes to be all given in terms of two amplitudes, one for total isospin $I = \frac{3}{2}$ and one for total isospin $I = \frac{1}{2}$. The amplitudes are given by the so-called scattering matrix whose matrix elements are obtained by evaluating the scattering operator S between incoming and outgoing states. The detailed theory of the scattering matrix will be given in Chapters 8 and 9. There we shall see that if all generators I_i of isospin rotations commute with the Hamiltonian operator of strong interactions H_{strong}, they also commute with the scattering operator S. Then the amplitudes do not depend on the I_3 components of the total isospin.

$$[I_i, S] = 0. \tag{22.33}$$

We therefore can use I_+ inside the matrix elements $\langle I, I_3|S|I, I_3\rangle$ to change I_3 to any allowed value $|I_3| \leq I$. From

$$\langle I, I_3|I_+S|I, I_3-1\rangle = \langle I, I_3|SI_+|I, I_3-1\rangle \tag{22.34}$$

it follows that

$$\begin{aligned}\langle I, I_3-1|S|I, I_3-1\rangle&\sqrt{(I+I_3)(I-I_3+1)}\\ = \langle I, I_3|S|I, I_3\rangle&\sqrt{(I+I_3)(I-I_3+1)}\end{aligned} \tag{22.35}$$

[see Eqs. (4.370), (4.374)]. Thus the diagonal matrix elements $\langle I, I_3|S|I, I_3+1\rangle$ are independent of I_3. Similarly one sees that the non-diagonal elements vanish. We therefore define the reduced scattering amplitude S^I of a given isospin I by the equation

$$\langle I, I_3'|S|I, I_3\rangle \equiv \delta_{I_3'I_3}S^I. \tag{22.36}$$

This statement is a special case of the Wigner-Eckart theorem (3.834) for the matrix elements of an arbitrary spherical tensor operator T_{I,I_3} of isospin I. Such a tensor operator is defined by the transformation law [compare (3.830)]

$$[I_i, T_{I,I_3}] = T_{I,I_3'}D^I(I_i)^{I_3'}{}_{I_3}, \tag{22.37}$$

where $D^I(I_i)_{I_3}{}^{I_3'}$ are the representation matrices of the generators I_i of the isospin rotation group. According to the Wigner-Eckart theorem, the matrix elements of a tensor operator between the representation states $|I, I_3\rangle$ are related by Clebsch-Gordan coefficients:

$$\langle I'', I_3''|T_{I',I_3'}|I, I_3\rangle = \langle I'', I_3''|I', I_3'; I, I_3\rangle\langle I''||T||I\rangle, \tag{22.38}$$

which account for the dependence on the quantum numbers I_3, I_3', I_3''. The matrix elements depend only on a few *reduced matrix elements* $\langle I''||T||I\rangle$ which are nonzero if the isospins I and I' can be coupled to I''. Within this definition, the scattering operator is trivial tensor operator of isospin zero where (22.38) reduces to (22.36).

Note that (22.36) is also a manifestation of Im Schur's Lemma, according to which a matrix commuting with an irreducible set of matrices must be proportional to the unit matrix.

As an application of (22.36), the scattering amplitudes for various pion-nucleon scattering processes are given by the following combinations of only two amplitudes, $S^{3/2}$ and $S^{1/2}$:

$$\begin{aligned}S_{\pi^+p\rightarrow\pi^+p} &= S^{3/2},\\ S_{\pi^+n\rightarrow\pi^+n} &= (1/3)S^{3/2} + (2/3)S^{1/2},\\ S_{\pi^0p\rightarrow\pi^0p} &= (2/3)S^{3/2} + (1/3)S^{1/2},\\ S_{\pi^+n\leftrightarrow\pi^0p} &= (\sqrt{2}/3)S^{3/2} - (\sqrt{2}/3)S^{1/2},\end{aligned}$$

$$\begin{aligned} S_{\pi^0 n\to\pi^0 n} &= (2/3)S^{3/2} + (1/3)S^{1/2}, \\ S_{\pi^+ p\to\pi^- p} &= (1/3)S^{3/2} + (2/3)S^{1/2}, \\ S_{\pi^0 n\leftrightarrow\pi^- p} &= (\sqrt{2}/3)S^{3/2} - (\sqrt{2}/3)S^{1/2}, \\ S_{\pi^- n\to\pi^- n} &= S^{3/2}. \end{aligned} \tag{22.39}$$

(22.40)

The $\leftrightarrow$ symbols in the charge exchange reactions exhibit time-reversal invariance. By taking the absolute squares of the amplitudes, we see that the cross sections must satisfy

$$\sigma_{\pi^- p\leftrightarrow n\pi^0} + 2\sigma_{\pi^0 p\to\pi^0 p} = \sigma_{\pi^+ p\to\pi^+ p} + \sigma_{\pi^- p\to\pi^- p}. \tag{22.41}$$

This is borne out by experiment.

22.4 SU(3)-Symmetry

In 1944, the set of fundamental particles was enriched by a particle which was a heavy neutral meson of mass ≈ 500 MeV with a lifetime of $\tau \approx 10^{-10}$ sec. It was called a *strange particle*[2] and is now called K^0. It is now known to decay mainly into π^+, π^- and has

$$\begin{aligned} m_{K^0} &\approx 497.72 \pm 0.07 \text{ MeV }, \\ \tau_{K^0} &\approx (0.8323 \pm 0.0022) \times 10^{-10}\text{sec}. \end{aligned} \tag{22.42}$$

In 1951, a charged partner of this particle was discovered which decays mostly into a μ^+ and a neutrino of the meson type, namely the K^+ meson. It has a mass and a lifetime

$$\begin{aligned} m_{K^+} &\approx 493.667 \pm 0.014 \text{ MeV }, \\ \tau_{K^+} &\approx (1.2371 \pm 0.0026) \times 10^{-8}\text{sec}. \end{aligned} \tag{22.43}$$

One later found also a K^- decaying into negatively meson and a neutrino with the same lifetime. In 1955 one discovered, moreover, that there are actually two K^0 mesons, now called K^0 and $\bar{K}^0$. These mesons could soon be produced abundantly in particle accelerators and it became possible to study their interactions with nucleons. In the course of this it was found that not only the mesons but also the nucleons possess strange partners. Moreover, if one assigned to the strange mesons a quantum number $S = 1$, called "strangeness", and to the strange partner f the baryons in the associate production $S = -1$, then strangeness is a conserved quantum number in a nuclear scattering process. If an ordinary non-strange meson such as a pion hits a nucleon, then out comes either a pion and a nucleon both of strangeness zero, or a strange meson with $S = 1$ together with a strange partner of the nucleon with $S = -1$. For example

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[2] M. Gell-Mann, Phys. Rev. *92*, 833 (1952); T. Nakano, K. Nishijima, Progr. Theor. Phys. *10*, 581 (1953).

$$\pi^- p \to \pi^- p \tag{22.44}$$

or

$$\pi^- p \begin{array}{l} \nearrow \\ \searrow \end{array} \begin{array}{l} K^0\Lambda^0, \\ K^+\Sigma^-, \end{array} \tag{22.45}$$

There are also associate production processes where two K's are produced in addition to a nucleon:

$$\pi^- p \to K^- K^0 p, \tag{22.46}$$

$$\pi^+ p \to K^+ \bar{K}^0 p. \tag{22.47}$$

These allow us to deduce the strangeness for K^+, K^- have the strangeness $S = 1, -1$, respectively.
By scattering further a strange meson K^- on a proton,

$$K^- p \to K^+ \Xi^-, \tag{22.48}$$

one is able to produce a new particle Ξ^- of strangeness $S = -2$. This particle is called *cascade* since it decays in a cascade like process with the first step

$$\Xi^- \to \Lambda^0 \pi^- \tag{22.49}$$

and the second steps

$$\Lambda^0 \to p\pi^-, \tag{22.50}$$

$$\pi^- \to \mu^- \bar{\nu}_\mu. \tag{22.51}$$

Note that in contrast to the production process, the decay of the strange particles violates strangeness. For instance:

$$\begin{array}{rcccc} & \Sigma^- & \to & \pi^- & n \\ S: & -1 & & 0 & 0. \end{array} \tag{22.52}$$

This violation, however, can be blamed on another interaction, the weak interaction, since the decay proceeds quite slowly, with a lifetime of roughly 10^{10} sec.

While non-strange particles have a charge

$$Q = N/2 + I_3, \tag{22.53}$$

where N is the total nucleon-number, the charge of strange particles is given by

$$Q = Y/2 + I_3, \tag{22.54}$$

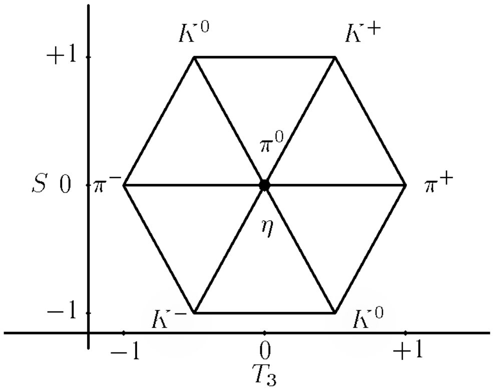

FIGURE 22.6 Pseudoscalar meson octet states associated with the pions. The same picture holds for the vector meson octet states with the replacement (22.58).

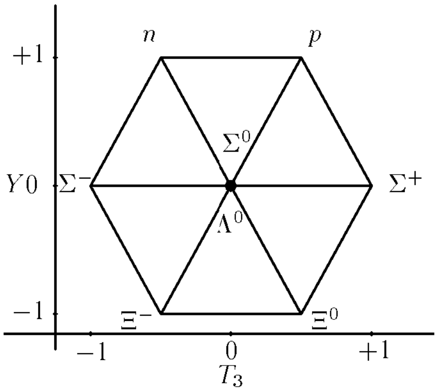

FIGURE 22.7 Baryon octet states associated with the nucleons.

with Y being defined as a convenient combination of N, and S, called hypercharge

$$Y \equiv N + S. \tag{22.55}$$

Gell-Mann plotted the known ordinary and strange pseudoscalar meson states in the I_3, Y plane and found the multiplet of eight particles shown in Fig. 22.6 (there and in subsequent similar plots the ket symbols $|\dots\rangle$ of the states are omitted). The center contains, beside the π^0-meson, another pseudoscalar neutral meson called the η meson. Its mass is

$$m_\eta = 548.8 \pm 0.6 \text{ MeV} \tag{22.56}$$

and it decays with a width

$$\Gamma \approx 1.05 \pm 0.15 \; keV \tag{22.57}$$

principally into $\gamma\gamma$ and $3\pi^0$. A ninth much heavier pseudoscalar meson $\eta'(958)$ of width 8.5 MeV known at that time did not fit into the scheme by having a larger mass and no partners.

Gell-Mann did the same thing with the spin 1 resonances of negative parity of the nine pseudoscalar particles, replacing

$$\begin{array}{lcl} K & \longrightarrow & K^*(892) \\ \pi & \longrightarrow & \rho(770) \\ \eta & \longrightarrow & \omega(783) \\ \eta' & \longrightarrow & \phi(1020) \end{array} \tag{22.58}$$

He continued to organize the nucleons and their strange partners in this way and found again an octet shown in Fig. 22.7 with the masses and lifetimes given in Table 22.1. Gell-Mann further noticed that there exists no similar regularity also

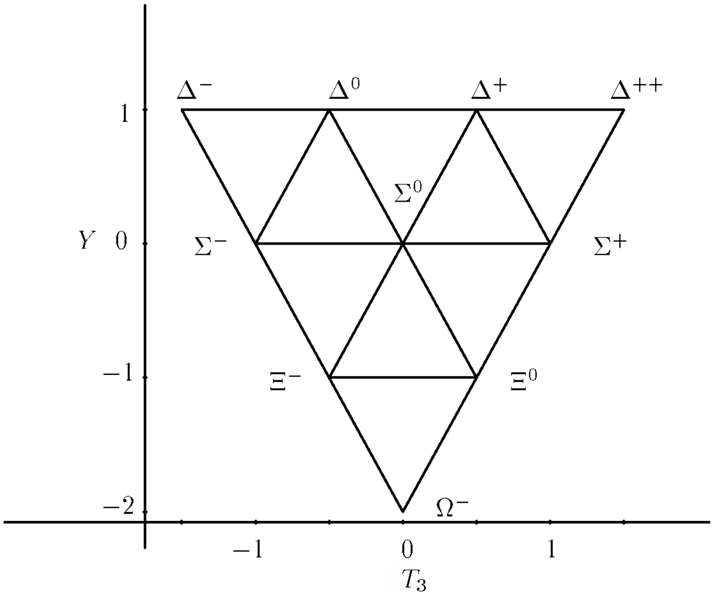

FIGURE 22.8 Baryon decuplet states associated with the first resonance of the nucleons.

TABLE 22.1 Masses and lifetimes of the octet states associated with the nucleons.

	m(MeV)	τ (10^{-10} sec)
p	938.2796± 0.0027	stable
n	939.5731± 0.0027	(898 ± 16) × 10^{10}
Σ^+	1189.37 ± 0.06	0.8 ± 0.004
Σ^-	1197.34 ± 0.05	1.482± 0.011
Σ^0	1192± 0.08	(5.8± 1.3) × 10^{10}
Λ^0	1115.60 ± 0.05	2.632 ± 0.020
Ξ^0	1314.9 ± 0.6	1.642 ± 0.015
Ξ^-	1321.32 ± 0.13	1.642 ± 0.015

for the most prominent excited states of the nucleon, the resonance $\Delta(1232)$ of mass 1232 MeV and width 115 ± 5 MeV and with charge states $-, 0, +, ++$ together with their strange partners $\Sigma(1385)$ of width $\approx$ 37 MeV and $\Xi(1530)$ of width $\approx$ 10 MeV. When he looked at the masses of these excited states he observed an about equal spacing when plotted in proportional to Y. When plotted in an I_3, Y system, the particles fill an equilateral triangle except for a missing lower corner. Starting from these observation he put forward the hypothesis that just as nuclear forces are independent under isospin rotations, which form the group of unitary matrices in two dimensions, they should also be approximately invariant under the most direct extension of this group, which includes the additional quantum number of strangeness. So he postulated an approximate invariance of the strong interactions under the the group of unitary matrices in three dimensions, SU(3). Since the masses splittings are much larger than in the former SU(2) multiplets, this symmetry is much more broken in nature then the isotopic symmetry.

In field theory, the group theoretic implications of SU(3) symmetry are studied by equipping the relativistic fields describing all paricles involved with an extra SU(3) subscript. First one intruduces a Dirac field with subscripts $\alpha = 1,\ 2,\ 3$:

$$\psi(x) -> \psi_\alpha(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \end{pmatrix}, \tag{22.59}$$

which changes under SU(3)-transformations by group elements from the fundamental three dimensional representation of SU(3), called 3. This fundamental property will be emphasized by calling such Dirac fields *quark fields*, and denoting them by $q_\alpha(x)$. Omitting the spacetime arguments, the transformation law is:

$$3: \quad q_\alpha \quad \longrightarrow \quad {U_\alpha}^\beta q_\beta, \qquad U \in \mathrm{SU}(3). \tag{22.60}$$

The hermitian adjoint of a quark field, $(q_\alpha)^\dagger \equiv (q^\dagger)^\alpha$ transforms according to the complex conjugate representation, called 3^*. To emphasize the different transformation behavior we write $[{U_\alpha}^\beta]^\dagger$ as ${(U^*)^\alpha}_\beta$ so that

$$3^*: \quad q^{\dagger\alpha} \quad \longrightarrow \quad {U^{*\alpha}}_\beta q^{\dagger\beta}, \qquad U \in \mathrm{SU}(3). \tag{22.61}$$

The unitary scalar product $q^\dagger q \equiv (q^\dagger)^\alpha q_\alpha$ is an invariant and the same thing is true for the contraction of q_α with any other particle field which transforms like $(q^\dagger)^\alpha$. For Dirac fields it is more convenient to work with the fields $\bar{q}(x) = q^\dagger(x)\gamma^0$ rather than $q^\dagger(x)$ because of their more favorable Lorentz transformation properties, in particular the Lorentz in variance of the scalar product $\bar{q}(x)q(x)$. Thus we shall work with conjugate quark fields

$$\bar{q}^\alpha = (\bar{q}^1, \bar{q}^2, \bar{q}^3). \tag{22.62}$$

The contraction $\bar{q}^\alpha q_\alpha$ is obviously invariant under Lorentz- *and* SU(3)-transformations:

$$\bar{q}^\alpha q_\alpha = \text{invariant} \tag{22.63}$$

We have seen in Eq. (5.296) that the charge-conjugate Dirac field is directly related to $\bar{q}$ by a similarity transformation of the Dirac indices, which for quark fields reads

$$q_C(x) = C\bar{q}^T(x). \tag{22.64}$$

The fields $\bar{q}$ annihilate antiparticles, and will therefore be referred to as *antiquark fields*, ignoring at this point the similarity transformation.

The traceless tensor field obtained from the direct product of q_α and $\bar{q}^\beta$

$$M_\alpha{}^\beta \equiv q_\alpha \bar{q}^\beta - \tfrac{1}{3}\delta_\alpha{}^\beta q_\gamma \bar{q}^\gamma \tag{22.65}$$

is, in general, a bilocal field containing $q_\alpha(\mathbf{x}, t)$ and $\bar{q}^\beta(\mathbf{x}', t)$ at different space points which are irrelevant to the present discussion and therefore omitted. This field forms an invariant 8-dimensional representation space of SU(3) which Gell-Mann identified with the 8 meson states described above. This octet representation is irreducible. This means that every state of it can be reached by performing group operations on an arbitrary single fixed state. Gell-Mann called the fields up, down, and strange quark fields and denoted them by u, d, s, i.e.

$$q_\alpha = \begin{pmatrix} u \\ d \\ s \end{pmatrix}. \tag{22.66}$$

Similarly for the antiquarks:

$$\bar{q}^\alpha = (\bar{u}, \bar{d}, \bar{s}). \tag{22.67}$$

He associated the octet fields (22.65) with the pseudoscalar mesons as shown in Fig. 22.9. The field $M_\alpha{}^\beta$ annihilates the corresponding particle, for example $\pi^+ \equiv M_1{}^2 = \bar{d}u$ annihilates the particle π^+. In contrast to isospin, the SU(3) symmetry is

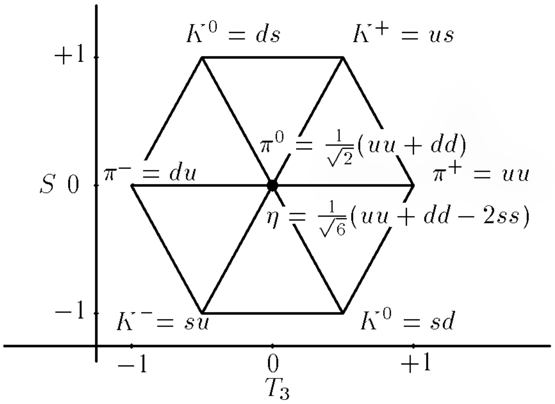

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FIGURE 22.9 Quark content of the pseudoscalar meson octet fields. The particle and quark symbols denote the *annihilation* parts of the corresponding fields.

strongly broken. The pion and the K mesons have quite different masses, 135 MeV and 490 MeV.

The operator which measures the third component of isospin , I_3, is the number operator

$$\hat{I}_3 = \frac{1}{2}[(\hat{N}_u - \hat{N}_d) - (\hat{N}_{\bar{u}} - \hat{N}_{\bar{d}})]. \tag{22.68}$$

Here and in the sequel we denote by $\hat{N}_{u,d,s}$ the total number operator of the u, d, s quarks and their antiparticles, respectively. Thus we have the commutation rules

$$-[\hat{N}_{u,d}, q_\alpha] = n_{u,d} q_\alpha, \quad \alpha(u, d, s) \tag{22.69}$$

with the eigenvalues

$$n_u = (1,0,0), \quad n_d = (0,1,0), \tag{22.70}$$

and similar relations between the number operators and the antiquarks $\bar{q}^\alpha = (\bar{u}, \bar{d}, \bar{s})$. The hypercharge of the mesons is given by

$$\hat{Y} = \frac{1}{3}[(\hat{N}_u + \hat{N}_d - 2\hat{N}_s) - (\hat{N}_{\bar{u}} + \hat{N}_{\bar{d}} - 2\hat{N}_{\bar{s}})], \tag{22.71}$$

where N_s counts the number of strange quarks, i.e., it is defined to have, for (u, d, s) and $(\bar{u}, \bar{d}, \bar{s})$, the eigenvalues $n_s = (0,0,1)$ and $(0,0,-1)$, respectively, with corresponding eigenvalues of $N_{\bar{s}}$ for the antiquarks.

The group SU(3) is a $3 \cdot 3 - 1 = 8$ parameter group. Its Lie algebra possesses 8 traceless hermitian generators which are conventionally denoted by $\lambda^a/2$ $(a = 1, \cdots, 8)$ with the 3×3 traceless hermitian matrices

$$\begin{aligned}
\lambda^1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\lambda^4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda^5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \\
\lambda^6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \lambda^7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda^8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
\end{aligned} \tag{22.72}$$

Note that they have the same trace orthonormality relations as the Pauli matrices:

$$\mathrm{tr}\,(\lambda^a \lambda^b) = 2\delta_{ab}. \tag{22.73}$$

It is easy to see that the 3×3 -matrices $U = e^{i\alpha_a \lambda^a/2}$ span the space to unitary 3×3 -matrices of unit determinant. The first three λ^a's are the direct extension of the σ^i-matrices of isospin into three dimensions.

The group structure is specified by the commutation rules of the generators

$$[\lambda^a, \lambda^b] = 2if_{abc}\lambda^c \tag{22.74}$$

where the structure constants f_{abc} are totally antisymmetric in abc, due to the Jacobi identity satisfied by the commutators. Their values are given in Table 22.4. Let G_a

Table 22.2 Structure Constants of SU(3). All elements not given in the table follow from the total antisymmetry.

abc	f_{abc}
123	1
147	1/2
156	-1/2
246	1/2
257	1/2
345	1/2
367	-1/2
458	$\sqrt{3}/2$
678	$\sqrt{3}/2$

be the operators in Hilbert space associated with these Lie algebra elements. They act on the three quark field operators of the fundamental representation as follows:

$$-\left[\hat{G}_a, q_\alpha\right] = (\lambda^a/2)_\alpha{}^\beta q_\beta. \tag{22.75}$$

An explicit operator expression for the generators can be given by assigning to the q-fields canonical commutation or anticommutation relations

$$[q_\alpha, q^{\dagger\beta}] = \delta_\alpha{}^\beta \tag{22.76}$$

Then we can express the generators $\hat{G}_i$ simply as follows [recall Section 2.5]

$$G_a = q^{\dagger\alpha}(\lambda^a/2)_\alpha{}^\beta q_\beta. \tag{22.77}$$

It is easy to see that these operators $\hat{G}^a$ have indeed the same commutation relation as the matrices $\lambda^a/2$:

$$[\hat{G}_a, \hat{G}_b] = i f_{abc} \hat{G}_c. \tag{22.78}$$

Besides these commutators, some calculations will involve the anticommutators of the λ^a-matrices. They are given by

$$\left\{\lambda^a, \lambda^b\right\} = 2 d_{abc} \lambda^c + (4/3)\delta_{ab} \tag{22.79}$$

where d_{abc} are completely symmetric in abc and have the nonzero matrix elements shown in Table 22.3.

Consider now antiquark fields transforming according to the the representation 3^* of SU(3). Under commutation with $\hat{G}_a$ the antiquark fields behaves as follows

$$-[\hat{G}_a, \bar{q}^\alpha] = -\bar{q}^\beta (\lambda^a/2)_\beta{}^\alpha = -(\lambda^{a*}/2)^\alpha{}_\beta \bar{q}^\beta. \tag{22.80}$$

The antiquark field have the same commutation rules as the quark fields, i.e., with the index notation $(\bar{q}^\dagger)_\alpha \equiv (\bar{q}^\alpha)^\dagger$,

$$[\bar{q}^\beta, \bar{q}^\dagger_\alpha] = \delta^\beta{}_\alpha. \tag{22.81}$$

TABLE 22.3 The symmetric couplings d_{abc}. All values not given explicitly are obtained from the total symmetry in *abc*.

abc	d_{abc}	*abc*	d_{abc}
118	$1/\sqrt{3}$	355	$1/2$
146	$1/2$	366	$-1/2$
157	$1/2$	377	$-1/2$
228	$1/\sqrt{3}$	448	$-1/2\ \sqrt{3}$
247	$-1/2$	558	$-1/2\sqrt{3}$
256	$1/2$	668	$-1/2\ \sqrt{3}$
338	$1/\sqrt{3}$	778	$-1/2\ \sqrt{3}$
344	$1/2$	888	$-1/\sqrt{3}$

The generators of SU(3) have for quark and antiquark fields therefore an operator form:

$$\hat{G}_a = q^\dagger(\lambda^a/2)q - \bar{q}^\dagger(\lambda^{a*}/2)\bar{q}. \tag{22.82}$$

The generator of the third component if isospin is

$$\begin{aligned}\hat{I}_3 = \hat{G}_3 &= q^\dagger(\lambda^3/2)q - \bar{q}^\dagger(\lambda^3/2)\bar{q} \\ &= \frac{1}{2}(u^\dagger u - d^\dagger d) - \frac{1}{2}(\bar{u}^\dagger\bar{u} - \bar{d}^\dagger\bar{d}).\end{aligned} \tag{22.83}$$

Similarly, the hypercharge is given by

$$\begin{aligned}\hat{Y} = \frac{2}{\sqrt{3}}\hat{G}_8 &= \frac{2}{\sqrt{3}}\left[q^\dagger(\lambda^8/2)q - \bar{q}^\dagger(\lambda^8/2)\bar{q}\right] \\ &= \frac{1}{3}\left[(u^\dagger u + d^\dagger d - 2s^\dagger s) - (\bar{u}^\dagger\bar{u} + \bar{d}^\dagger\bar{d} - 2\bar{s}^\dagger\bar{s})\right],\end{aligned} \tag{22.84}$$

and the charge by

$$\begin{aligned}\hat{Q} &= Y/2 + I_3 \\ &= \frac{1}{3}\left[(2u^\dagger u - d^\dagger d - s^\dagger s) - (2\bar{u}^\dagger\bar{u} - \bar{d}^\dagger\bar{d} - \bar{s}^\dagger\bar{s})\right].\end{aligned} \tag{22.85}$$

The raising and lowering of the third component is done with the operators

$$\begin{aligned}\hat{I}_\pm &= \tfrac{1}{2}\left[q^\dagger\lambda^{1\pm i2}q - \bar{q}^\dagger(\lambda^{1\pm i2})^*\bar{q}\right] \\ &= \left\{\begin{array}{ccc} u^\dagger d & - & \bar{d}^\dagger\bar{u} \\ d^\dagger u & - & \bar{u}^\dagger\bar{d}\end{array}\right\},\end{aligned} \tag{22.86}$$

where $\lambda^{1\pm i2}$ is a short notation for $\lambda^1 \pm i\lambda^2$. A pair of operators which raise and lower the hypercharge by a unit (thereby also raising and lowering I_3 by half a unit) is[3]

$$\begin{aligned} \hat{V}_{\pm} &= \tfrac{1}{2}\left[q^\dagger\lambda^{4\pm i5}q - \bar{q}^\dagger(\lambda^{4\pm i5})^*\bar{q}\right] \\ &= \left\{\begin{array}{ccc} s^\dagger u & - & \bar{s}^\dagger\bar{u} \\ u^\dagger s & - & \bar{u}^\dagger\bar{s} \end{array}\right\}. \end{aligned} \tag{22.87}$$

The effect of these operators on the quark and antiquark states $|q_\alpha\rangle$ (created by the operators $(q^\dagger)^\alpha$ when acting on the vacuum $|0\rangle$) is illustrated in Fig. 22.10 [this being the analog to the illustration in Fig. 3.3]. Note that there exists a related pair of operators which raise and lower hypercharge by a unit while acting oppositely to $V_\pm$ in the isospin:

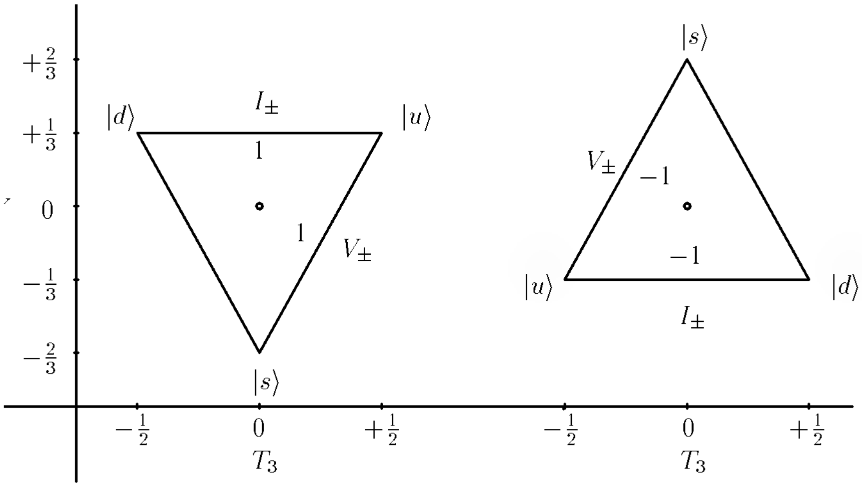

FIGURE 22.10 Effect of raising and lowering operators on quark and antiquark states. Here and in the subsequent weight diagrams the ket symbols of the states are omitted.

$$\begin{aligned} \hat{U}_{\pm} &= \tfrac{1}{2}\left[q^\dagger\lambda^{6\pm i7}q - \bar{q}^\dagger(\lambda^{6\pm i7})^*\bar{q}\right] \\ &= \left\{\begin{array}{ccc} s^\dagger d & - & \bar{s}^\dagger\bar{d} \\ d^\dagger s & - & \bar{d}^\dagger\bar{s} \end{array}\right\}. \end{aligned} \tag{22.88}$$

These, however, will play no role in the future discussion.

Consider now the composite states associated with the product representation $3 \times \bar{3}$ of a quark and an antiquark assigned to the pseudoscalar mesons in (22.65). The quantum numbers I_3 and Y are additive so that the quantum numbers of the mesons octet can be found by vector addition, i.e. by placing the $\bar{3}$ diagram with the (I_3, Y) origin once on each state of the 3 diagram and adding up the vectors as shown in Fig. 22.11. In the theory of group representations the vectors $|I_3, Y\rangle$ of the quarks and the antiquarks are referred to as the *fundamental weights*. Using the raising and lowering operators $I_\pm, V_\pm$ it is easy to find all states of an irreducible representation starting out from any fixed state. For instance, the operators $\hat{I}_+$ to the particle state $|\pi^-\rangle = |d\bar{u}\rangle$, we find

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[3] Note that there exists a third component to the operators V_{pm}, $V_3 = \frac{1}{2}(u^\dagger u - s^\dagger s) - \frac{1}{2}(\bar{u}^\dagger\bar{u} - \bar{s}^\dagger\bar{s})$, which commutes with $V_\pm$ in the same way as the isospin operators. The three operators form the so-called V-spin subgroup of SU(3). A similar thing holds for the $U_\pm$ operators of (22.88) with $U_3 = \frac{1}{2}(d^\dagger d - s^\dagger s) - \frac{1}{2}(\bar{d}^\dagger\bar{d} - \bar{s}^\dagger\bar{s})$.

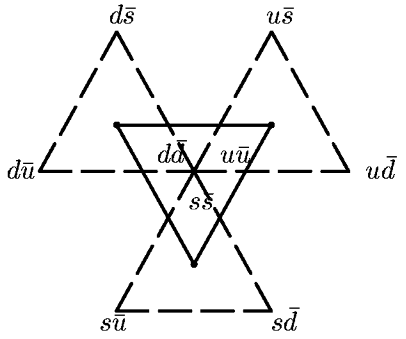

FIGURE 22.11 Adding the fundamental weights in product representation space of 3 and $\bar{3}$ vectors.

$$\hat{I}_+|\pi^-\rangle = |\bar{u}u - \bar{d}d\rangle \equiv \sqrt{2}|\pi^0\rangle, \tag{22.89}$$

and further

$$\hat{I}_+|\pi^0\rangle = -\sqrt{2}|\bar{d}u\rangle \equiv -\sqrt{2}|\pi^\dagger\rangle. \tag{22.90}$$

Similarly, applying V_+ to $|\pi^-\rangle = |\bar{u}d\rangle$ gives

$$\hat{V}_+|\pi^-\rangle = -|\bar{s}s\rangle = |K^0\rangle. \tag{22.91}$$

By applying $\hat{V}_+$ to $|\bar{K}_0\rangle$ we find

$$\hat{V}_+|\bar{K}^0\rangle = |\bar{u}u - \bar{s}s\rangle. \tag{22.92}$$

This state has the same (I_3, Y) quantum numbers as $|\pi^0\rangle$ but is not an eigenstate of total isospin I^2. Such a state is given by

$$|\eta\rangle = \sqrt{\tfrac{1}{6}}|\bar{u}u + \bar{d}d - 2\bar{s}s\rangle \tag{22.93}$$

so that $\hat{V}_+|\bar{K}^0\rangle$ can be decomposed into a π^0 and an η state as follows:

$$\begin{aligned} \hat{V}_+|\bar{K}^0\rangle &= \tfrac{1}{2}|\bar{u}u - \bar{d}d\rangle + \tfrac{1}{2}|\bar{u}u + \bar{d}d - 2\bar{s}s\rangle \\ &= \sqrt{\tfrac{1}{2}}|\pi^0\rangle + \sqrt{\tfrac{3}{2}}|\eta\rangle. \end{aligned} \tag{22.94}$$

It has become customary (de Swart convention[4]) to change the phases to the $\bar{q}$ states so that the matrix elements of $I_\pm$ and $V_\pm$ are all positive. This is achieved by changing the phases of the states of the representation 3^* as shown in Fig. 22.12. For

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[4] J.J. de Swart, Rev. Mod. Phys. *35*, 916 (1963).

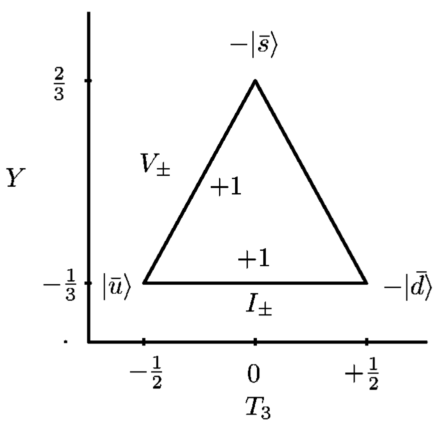
$-|\bar s\rangle$
$\frac{2}{3}$
Y
$V_\pm$
$+1$
$+1$
$-\frac{1}{3}$
$|\bar u\rangle$
$-|\bar d\rangle$
$I_\pm$
$-\frac{1}{2}$
0
$+\frac{1}{2}$
T_3

FIGURE 22.12 The states of the $\bar 3$-representation with de Swart phases.

the SU(3) representation matrices U^*, these phase changes on the states correspond to a similarity transformation. The new matrices will be denoted by $\bar U$:

$$U^* \longrightarrow \bar U \tag{22.95}$$

Correspondingly, we shall say that the antiquark fields $\bar q$ after the phase changes transform according to the $\bar 3$ representation.

The phases of all higher representations are adjusted accordingly. The meson octet states associated with the product of 3 and $\bar 3$ states are shown in Fig. 22.13. As a check we calculate a couple of phases:

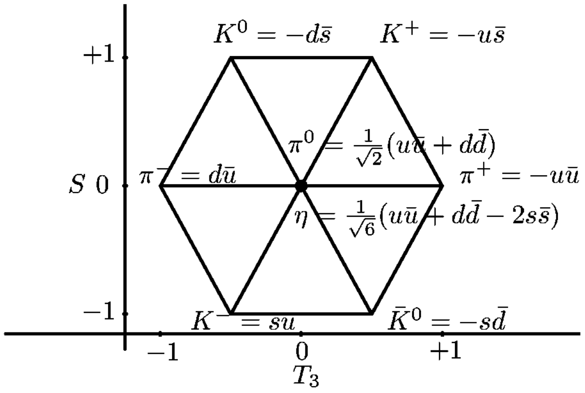
$K^0 = -d\bar s$
$K^+ = -u\bar s$
$+1$
$\pi^0 = \frac{1}{\sqrt 2}(u\bar u + d\bar d)$
S 0
$\pi^- = d\bar u$
$\pi^+ = -u\bar u$
$\eta = \frac{1}{\sqrt 6}(u\bar u + d\bar d - 2s\bar s)$
-1
$K^- = su$
$\bar K^0 = -s\bar d$
-1
0
$+1$
T_3

FIGURE 22.13 The quark-antiquark content of the meson octet meson states with de Swart phase convention.

$$\begin{aligned}\hat V_+|\pi^0\rangle &= \hat V_+\sqrt{\tfrac{1}{2}}|\bar u u - \bar d d\rangle\\ &= -\sqrt{\tfrac{1}{2}}|\bar s u\rangle = \sqrt{\tfrac{1}{2}}|K^+\rangle\end{aligned} \tag{22.96}$$

and

$$\hat{V}_+|K^-\rangle = \hat{V}_+|-\bar{d}s\rangle = -|\bar{d}u\rangle = |\pi^0\rangle, \tag{22.97}$$

which are indeed positive.

Note that these quark-antiquark states can also be obtained by forming certain combinations of λ^a-matrices and sandwiching them between the creation operator parts of the quark and antiquark fields

$$q^{\dagger\alpha} = (u^\dagger, d^\dagger, s^\dagger), \quad (\bar{q}^\dagger)_\alpha = (\bar{u}^\dagger, \bar{d}^\dagger, \bar{s}^\dagger), \tag{22.98}$$

and applying them to the vacuum. The creation operators of the meson octet states are

$$M^\dagger{}_a = q^\dagger(\lambda^a/\sqrt{2})\bar{q}^\dagger, \tag{22.99}$$

with the combinations indicated in Fig. 22.14. These combinations of λ^a indices are

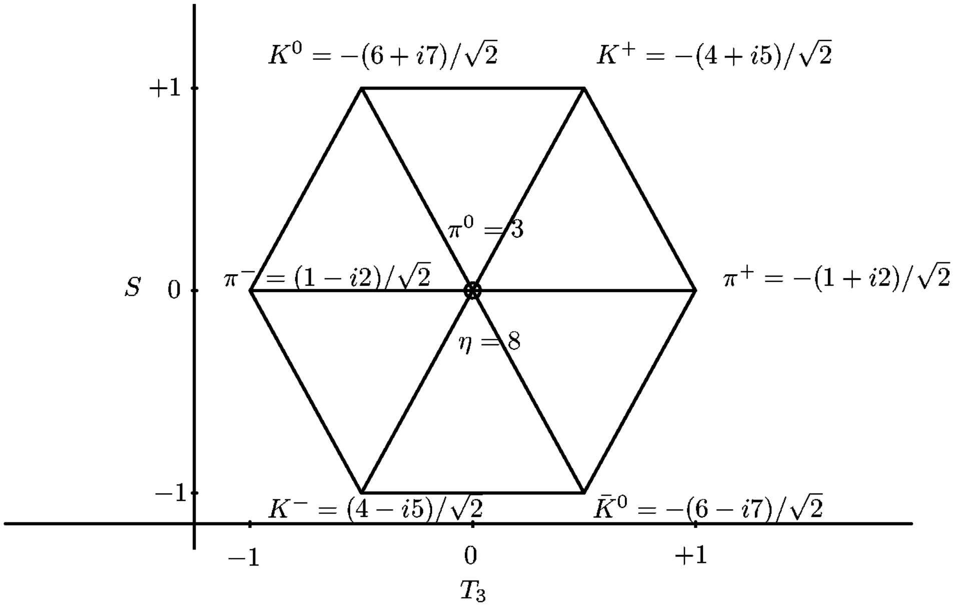

FIGURE 22.14 Combination of indices a in the pseudoscalar octet field $M^\dagger{}_a$ of (22.99). Here $-(1 \pm i2)/\sqrt{2}$ stands for $-(M^\dagger{}_1 \pm iM^\dagger{}_2)/\sqrt{2}$.

often used to specify octet states instead of the quark content. Any hermitian octet operator $\hat{O}_a$ (for instance $\hat{G}_a$ itself and $M^\dagger{}_a$) with the indices $-(1+i2)/\sqrt{2}$ adds to a given state the quantum numbers of a π^+. Let us verify the de Swart phases of the assignments in Fig. 22.14 by applying $\hat{I}_\pm, \hat{V}_\pm$ to the meson states $|M_a\rangle = M^\dagger{}_a|0\rangle$ with the above index combinations. Using the commutation rules

$$[\hat{G}_a, M^\dagger{}_b] = if_{abc}M^\dagger{}_c \tag{22.100}$$

we have, for example,

$$\begin{aligned}
[I_+, {M^\dagger}_{\pi^-}] &= \sqrt{2} f_{123} {M^\dagger}_3 = \sqrt{2} {M^\dagger}_{\pi^0}, \\
[I_+, {M^\dagger}_{\pi^0}] &= i\sqrt{\tfrac{1}{2}} f_{123}(-{M^\dagger}_2 + i{M^\dagger}_1) = {M^\dagger}_{\pi^+}, \qquad (22.101) \\
[I_+, {M^\dagger}_{K^0}] &= (f_{174} {M^\dagger}_4 - f_{165} {M^\dagger}_5) = -\sqrt{2} {M^\dagger}_{K^+}.
\end{aligned}$$

There is another simple way of constructing an octet representation of SU(3) from quark states without the use of antiquarks. By applying the product of three fields $q^\dagger_\alpha q^\dagger_\beta q^\dagger_\gamma$ at three different places[5] to the vacuum one obtains 27 states. If these are decomposed into the irreducible contents of SU(3) they lead to the following multiplets

$$3 \times 3 \times 3 = 10 + 8 + 8 + 1. \qquad (22.102)$$

The octet states can be identified with the nucleon octet states. In the decuplet there are doubly charged non-strange states which can be identified with the first nucleon resonance $\Delta(1236)$. It is therefore suggestive to identify the other 10 states with the strange partners of this resonance. At the time when Gell-Mann proposed this identification he could only match 9 of the decuplet states with known particles and resonances. There was one more state of strangeness 2 at the bottom of the weight diagram to be constructed in Fig. 22.17 which closes it to a triangle. Since the masses within the two rows are almost degenerate and since they grow from row to row by about the same amount

$$\begin{aligned}
m_\Delta - m_{\Sigma^*} &\approx -150, \\
m_{\Sigma^*} - m_{\Xi^*} &\approx -145,
\end{aligned}$$

with the masses given in units MeV, Gell-Mann extrapolated the mass of the tenth particle to be

$$\begin{aligned}
M &\approx M_\Delta + 3(M_\Sigma - M_\Delta) \\
&\approx 1232 + 3 \cdot 1567 \approx 1682. \qquad (22.103)
\end{aligned}$$

He therefore postulated the existence of a particle with this mass, a negative charge, and a hypercharge -2 as it resulted from the three quark content of the states and called the particle Ω^-. This particle was found in 1964 at a mass of 1675 ± 8 Mev. It was a triumph of the approximate SU(3) symmetry hypothesis and the 10 assignment of the excited nucleons and their strange partners.

Let us explicitly construct the irreducible representations contained in the product $3 \times 3 \times 3$ and assign them to physical states. We perform the multiplication successively

$$3 \times 3 \times 3 = 3 \times (3 \times 3). \qquad (22.104)$$

---

[5] This assumption of different place points is necessary to get all 27 states for otherwise some states will coincide due to particle identity.

The product of two states 3 × 3 is easily reduced to

$$3 \times 3 = 6 + \bar{3}. \tag{22.105}$$

To see this we write down the antisymmetric and symmetric combinations as shown in Fig. 22.15. The first is a 6-representation, the second transforms in the same way as an antiquark representation $\bar{3}$. As before we have assigned the phases to satisfy the de Swart convention. After forming these products we continue the multiplication.

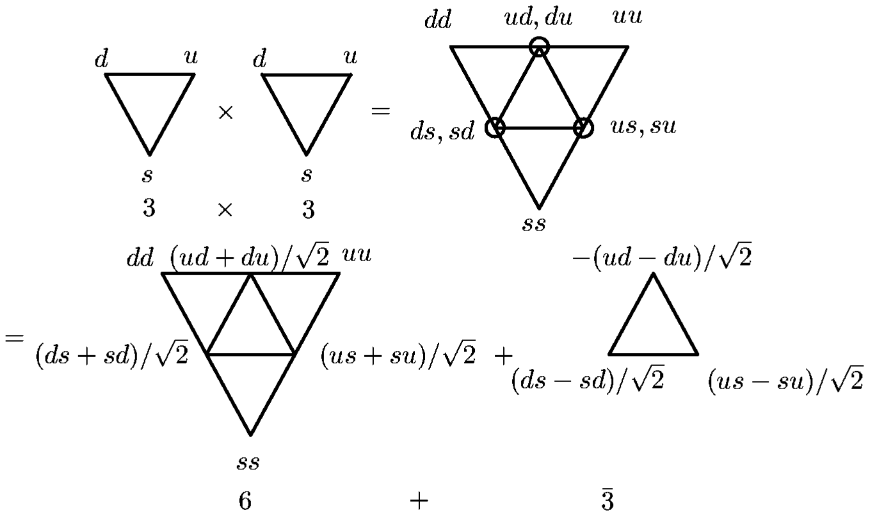

FIGURE 22.15 The quark content in the reduction of the product $3 \times 3 = 6 + \bar{3}$.

$$3 \times 3 \times 3 = 3 \times (6 + \bar{3}) = 3 \times 6 + 3 \times \bar{3} \tag{22.106}$$

Let us now form 3 × 6 and $3 \times \bar{3}$. The product $3 \times \bar{3}$ has been calculated before in terms of quark-antiquark states

$$3 \times \bar{3} = 8 + 1. \tag{22.107}$$

Now the octet states contain three quarks as shown in Fig. 22.16. The octet states can be identified with the nucleons and their strange partners.

The singlet state $|\Lambda_s\rangle$ is the completely antisymmetric combination of uds states:

$$|\Lambda_s\rangle = \frac{1}{\sqrt{3!}}(|uds\rangle + |dsu\rangle + |sud\rangle + |dus\rangle + |sdu\rangle + |usd\rangle). \tag{22.108}$$

The proton state is

$$|p\rangle = \frac{1}{\sqrt{2}}|u(ud - du)\rangle. \tag{22.109}$$

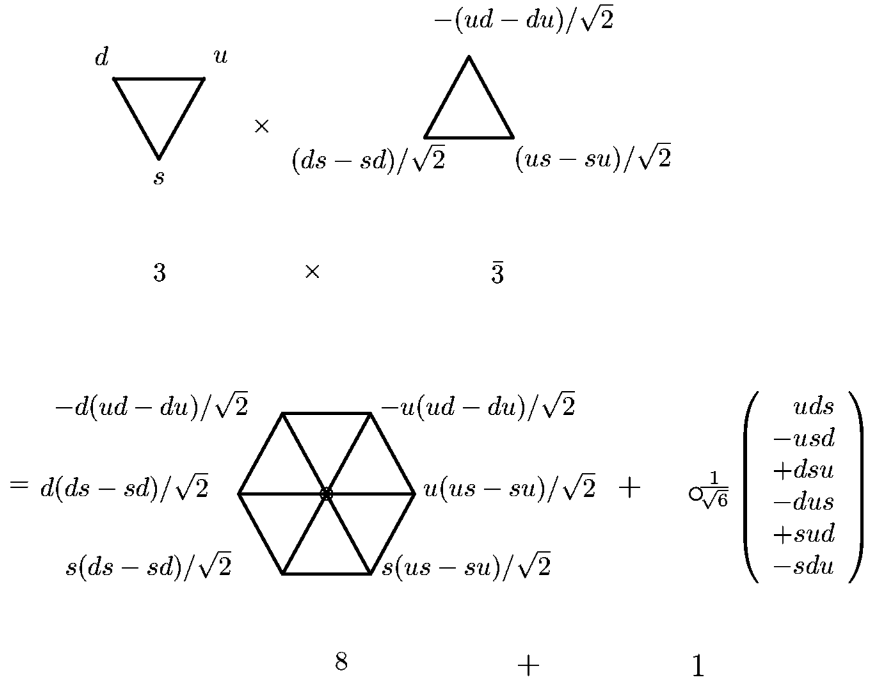

FIGURE 22.16 The octet and singlet states obtained from $3 \times \bar{3}$ in the product space of tree-quarks.

The state $|\Sigma^0\rangle$ in the octet is found by applying $\hat{I}_-$ to the right most state $|\Sigma^{\dagger}\rangle = -|u(us-su)\rangle$ thereby obtaining

$$|\Sigma^0\rangle = -\frac{1}{2}|d(us-su)+u(ds-sd)\rangle. \tag{22.110}$$

The isosinglet state $|\Lambda^0\rangle$ is obtained by applying $\hat{V}^-$ to $|p\rangle = |u(ud-du)\rangle/\sqrt{2}$ and separating the result into a linear combination of $|\Sigma^0\rangle$ and an orthogonal state which must be $|\Lambda^0\rangle$. First we have

$$\hat{V}^-|p\rangle = \sqrt{2}\frac{1}{2}|sud+usd-sdu-uds\rangle. \tag{22.111}$$

The scalar product with $|\Sigma^0\rangle$ gives

$$\langle\Sigma^0|\hat{V}^-|p\rangle = \frac{1}{\sqrt{2}}. \tag{22.112}$$

Hence we rewrite

$$V^-|p\rangle = \sqrt{2}\left(\tfrac{1}{2}|\Sigma^0\rangle + \tfrac{\sqrt{3}}{2}|\Lambda^0\rangle\right) \tag{22.113}$$

and identify

$$|\Lambda^0\rangle \equiv -\sqrt{1/12}|u(ds-sd)-d(us-su)-2s(ud-du)\rangle. \tag{22.114}$$

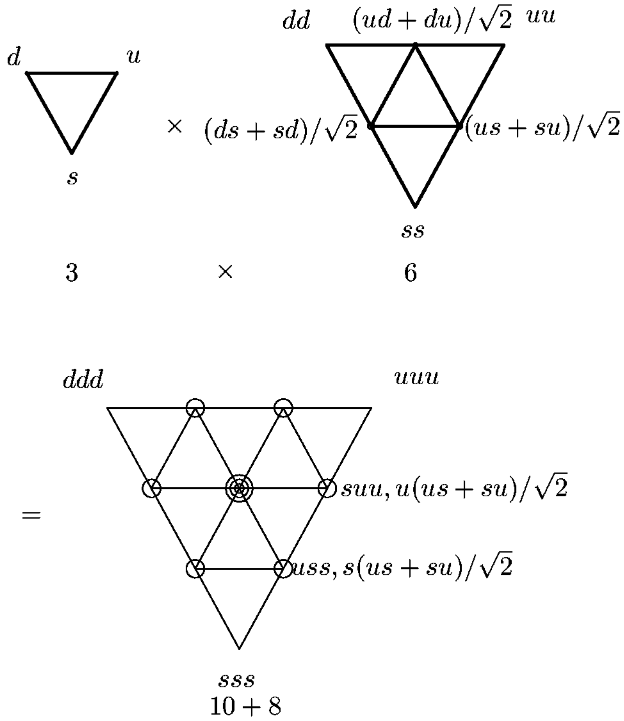

FIGURE 22.17 The irreducible three-quark states 10 and 8 in the product 3×6 (the symbol $(\ldots)_s$ denotes complete symmetrization).

Consider now the product 3×6. It gives the states shown in Fig. 22.17. The state $|uuu\rangle$ is identified with the 1232 MeV resonance $\Delta^{++}(1232)$ of isospin and parity $3/2^{\dagger}$. By applying the operators $I_\pm$ and $V_\pm$ to $|uuu\rangle$ we find the ten decuplet states

$$
\begin{array}{lcl}
|\Delta^{++}\rangle & = & |uuu\rangle \\
|\Delta^{+}\rangle & = & \sqrt{\frac{1}{3}}\ |uud + udu + duu\rangle \\
|\Delta^{0}\rangle & = & \sqrt{\frac{1}{3}}\ |udd + dud + udd\rangle \\
|\Delta^{-}\rangle & = & |ddd\rangle \\
|\Sigma^{+}\rangle & = & \sqrt{\frac{1}{3}}\ |uus + usu + suu\rangle \\
|\Sigma^{0}\rangle & = & \sqrt{\frac{1}{6}}\ |uds + usd + dsu + dus + sud + sdu\rangle \\
|\Sigma^{-}\rangle & = & \sqrt{\frac{1}{3}}\ |dds + dsd + sdd\rangle \\
|\Xi^{0}\rangle & = & \sqrt{\frac{1}{3}}\ |uss + sus + ssu\rangle \\
|\Xi^{-}\rangle & = & \sqrt{\frac{1}{6}}\ |dss + sds + ssd\rangle \\
|\Omega^{-}\rangle & = & |sss\rangle
\end{array}
$$

In addition to this decuplet, there is a further octet of particle states which can alternatively be assigned to the nucleon octet. Its quark states are found by constructing one state, say the proton, and applying the operators $I_\pm, V_\pm$ to it. The proton state is found by linearly composing $|uud\rangle$ and $|u(ud+du)\rangle/\sqrt{2}$ so that the result is orthogonal to $|\Delta^{+}\rangle$ in (22.115) and to $|p\rangle$ of (22.109):

$$|p'\rangle = \sqrt{\tfrac{1}{6}}|u(ud+du) - 2uud\rangle. \qquad (22.115)$$

The prime in $|p'\rangle$ indicates the different quark wave function with respect to (22.109). All other octet states associated with $|p'\rangle$ are then obtained by applying to it $I_\pm, V_\pm$, for instance

$$|n'\rangle = \hat{I}_-|p'\rangle = \sqrt{\tfrac{1}{2}}|d(ud-du)\rangle. \tag{22.116}$$

As a first test of the octet assignment we calculate the mass differences within the nucleon octet assuming that the mass operator transforms like an SU(3) singlet plus a form which behaves like a neutral isosinglet member of an octet, i.e., like η. Fortunately, the Glebsch-Gordan coefficients for the matrix elements

$$\langle 8_a|8_b|8_c\rangle \tag{22.117}$$

are already in our position. They are of two types and given by the traces $\mathrm{tr}\,([\lambda^a,\lambda^b]\lambda^c) = f_{abc}$ and $\mathrm{tr}\,(\{\lambda^a\lambda^b\}\lambda^c) = d_{abc}$. The first is antisymmetric, the second symmetric in abc. We therefore expand

$$\langle 8_a|8_b|8_c\rangle = Fif_{abc} + Dd_{abc}, \tag{22.118}$$

where F and D are two unknown irreducible matrix elements. To relate these to particles, we only have to multiply them with the SU(3)-polarization vectors $\epsilon_a(m)$ of the particles whose assignments are clear from Fig. (22.14). For instance

$$\epsilon_a(\pi^+) = -\frac{1}{\sqrt{2}}(1,i,0,0,0,0,0,0). \tag{22.119}$$

Then we have between particles

$$\langle 8m_2|8m|8m_1\rangle = \epsilon_a^*(m_2)\epsilon_b^*(m)(Fif_{abc} + Dd_{abc})\epsilon_c(m_1). \tag{22.120}$$

We may also write

$$\langle 8m_2|8m|8m_1\rangle = Fif_{m_2*m^*m_1} + Dd_{m_2^*m^*m_1}, \tag{22.121}$$

with obvious notation. The matrix associated with the $b = 8 \hat{=} \eta$ component are supposed to explain three mass differences. Two of them may be used to determine the two irreducible matrix elements F and D. The symmetry breaking will then allows us to derive one relation between the masses. Using the values of f_{abc} and d_{abc} with $b = 8$ from Table 22.3 we have for the distances of the masses from some common SU(3) singlet mass m_{sg}

$$\begin{array}{llllllll}
\Delta m_N & = & \langle p|8_\eta|p\rangle & = & Ff_{485} + Dd_{484} & = & F\sqrt{3}/2 - D/2\sqrt{3}, \\
\Delta m_\Sigma & = & \langle \Sigma^+|8_\eta|\Sigma^+\rangle & = & Dd_{181} & = & D/\sqrt{3}, \\
\Delta m_\Lambda & = & \langle \Lambda^0|8_\eta|\Lambda^0\rangle & = & Dd_{888} & = & -D/\sqrt{3}, \\
\Delta m_\Xi & = & \langle \Xi^0|8_\eta|\Xi^0\rangle & = & Ff_{687} + Dd_{686} & = & -F\sqrt{3}/2 - D/2\sqrt{3}.
\end{array} \tag{22.122}$$

Using these equations we readily find that the common singlet mass is

$$m_{sg} = \tfrac{1}{2}(m_\Sigma + m_\Lambda) = \tfrac{1}{2}(m_N + m_\Xi) + \tfrac{1}{4}(m_\Sigma - m_\Lambda), \tag{22.123}$$

so that the masses have to satisfy the famous Gell-Mann Okubo relation

$$\tfrac{1}{2}(m_N + m_\Xi) = \tfrac{1}{4}(3m_\Lambda + m_\Sigma). \tag{22.124}$$

It holds reasonably well, the left-hand side being approximately equal to 1.128 GeV the right-hand side 1.134 GeV.

For the decuplet, the same ansatz reproduces the equal mass splittings between the rows which had led Gell-Mann to his prediction of the Ω-meson.

For the pseudoscalar meson octet the relative mass splitting is very large and the mass relation cannot be expected to be as good as for the baryon octet. If we use, however, the square masses, it is nevertheless in surprisingly good agreement with experiment:

$$m_K^2 = \tfrac{1}{4}(3m_\eta^2 + m_\pi^2). \tag{22.125}$$

The left-hand side is equal to 0.25 GeV^2, the right-hand side 0.23 GeV^2. An argument for using square-masses is that, in contrast to the fermion Lagrangian, the boson Lagrangian has a mass term proportional to m^2.

The vector meson octet has a smaller relative mass splitting and the mass relation should be good. If we insert, however, the experimental masses

$$m_{K^*}^2 = \tfrac{1}{4}(3m_\omega^2 + m_\rho^2). \tag{22.126}$$

there is a bad surprise: The left-hand side is equal to 0.80 GeV^2 while the right-hand side 0.61 GeV^2. This disagreement can be resolved[6] by postulating that the symmetry breaking part of the Lagrangian mixes the isosinglet octet state with the SU(3) singlet state. This is always possible with the symmetry breaking transforming like an η-meson. Specifically, if ω_0, ϕ_0 denote the SU(3) states, the physical particles can be

$$\begin{aligned} \omega &= \cos\theta\omega_0 - \sin\theta\phi_0 \\ \phi &= \sin\theta\omega_0 + \cos\theta\phi_0. \end{aligned} \tag{22.127}$$

with some unknown mixing angle θ. The symmetry breaking Lagrangian can contain the mass terms

$$\mathcal{L}_{\text{symm br}} = -m_8^2\omega_0^2 - m_1^2\phi_0^2 - m_{18}^2\phi_0\omega_0 + \ldots, \tag{22.128}$$

with some SU(3) octet, singlet, and mixing mass parameters and the associated SU(3) fields. The octet mass parameter is determined from the Gell-Mann Okubo relation (22.126) as

$$m_8 = 930 \text{ MeV}. \tag{22.129}$$

Between the physical states (22.127) this becomes diagonal if the mixing angle θ is given by

$$\theta = \frac{1}{2}\arctan\frac{m_{18}^2}{m_9^2 - m_1^2}. \tag{22.130}$$

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[6] J.J. Sakurai, Phys. Rev. Letters *9*, 472 (1962).

and the diagonal masses are

$$m_\omega^2 = \tfrac{1}{2}(m_8^2 + m_1^2) - \tfrac{1}{2}[(m_8^2 - m_1^2)^2 - m_{18}^4] \tag{22.131}$$

$$m_\phi^2 = \tfrac{1}{2}(m_8^2 + m_1^2) + \tfrac{1}{2}[(m_8^2 - m_1^2)^2 - m_{18}^4] \tag{22.132}$$

From the experimental numbers we determine the parameters

$$m_{18} \approx 0.65 \text{ MeV}, \quad \cos\theta \approx 0.77. \tag{22.133}$$

The mixing angle can be tested by experiment since it determines the decay rate of the processes

$$\phi \to K^+K^-. \tag{22.134}$$

which occurs with a width 2.2 MeV. Since the vector meson has spin 1, the pseudoscalar kaons must come out in a p-wave. Their orbital wave function is therefore antisymmetric. But for bosons the total wave function must be symmetric which implies that the SU(3) quantum numbers have to be coupled antisymmetrically. This, however, excludes the SU(3)-singlet part of ϕ from the decay (since its coupling would be proportional to δ_{ab} in the SU(3)-indices of the pseudoscalar mesons. The amplitude for the decay is therefore proportional to the SU(3) Clebsch-Gordan coefficient $\cos\theta(8_{\omega_0}|8_{K^+}|8_{K^-})\propto\cos\theta\langle 0,0|\tfrac{1}{2},\tfrac{1}{2},-\tfrac{1}{2}\rangle f_{845} = \cos\theta\times(1/\sqrt{2})\times(\sqrt{3}/2)$. This is to be compared with the decay $\rho^0 \to \pi^+\pi^-$ whose amplitude is proportional to $(8_{\rho^0}|8_{\pi^-}|8_{\pi^+})\propto\langle 1,0|1,1;1,-1\rangle f_1 23 = (1/\sqrt{2}) \times 1$. Taking the squares we find the ratio

$$\left|\frac{S(\phi \to K^+K^-)}{S(\rho^0 \to \pi^+\pi^-)}\right|^2 = \frac{3}{4}\cos^2\theta \approx 0.44. \tag{22.135}$$

The decay rates contain a phase space factor

$$\Gamma \propto \frac{q^3}{M^2}, \tag{22.136}$$

where q is the momentum of the emerging pseudoscalar mesons and M the mass of the decaying vector meson. In the processes at hand we have $q_K \approx 127, M_\phi \approx 1020$, $q_\pi \approx 359, M_\rho \approx 770$ MeV so that the phase space factors are 0.0020 MeV and 0.078 MeV, respectively. Together with (22.135) this gives the ratio of decay rates

$$\left|\frac{\gamma(\phi \to K^+K^-)}{\gamma(\rho^0 \to \pi^+\pi^-)}\right|^2 \approx 0.011. \tag{22.137}$$

The experimental ratio is

$$\left|\frac{\gamma(\phi \to K^+K^-)}{\gamma(\rho^0 \to \pi^+\pi^-)}\right|^2_{exp} \approx 0.014, \tag{22.138}$$

in reasonable agreement with SU(3) symmetry.

For the pseudoscalar mesons the same type of mixing can occur between η- and η'- mesons. However, since their mass difference is relatively large compared to that between ω and ϕ their mixing angle is much smaller which explains why no mixing was needed to satisfy their Gell-Mann Okubo relation (22.125).

As a further test of the octet assignment we may calculate branching ratios for the decay of the decuplet resonances in the nucleon and the meson octets. Also here the agreement with experimental data is reasonably good.

22.5 New Quarks

Recently discovered particles and the theoretical attempts to explain their interactions and decay properties suggest the existence of more quarks, a *charmed quark* called c, a *top quark* called t, and a *bottom quark* called b. It is tempting to try and incorporate these quarks into the above broken symmetry considerations and extend the basic quark antiquark SU(3) multiplet by these additional quarks to higher multiplets with an even larger broken symmetry group. This has led to reasonable particle classifications only if one includes the lightest of the additional quarks, the charmed quark c. The four quarks u, d, s, c may be considered as the fundamental representation 4 of an internal SU(4) symmetry group, with the antiquarks transforming according to $\bar{4}$. The weight diagram, is three-dimensional and contains an additional "charm" axis labeled by C in Fig. 22.18.

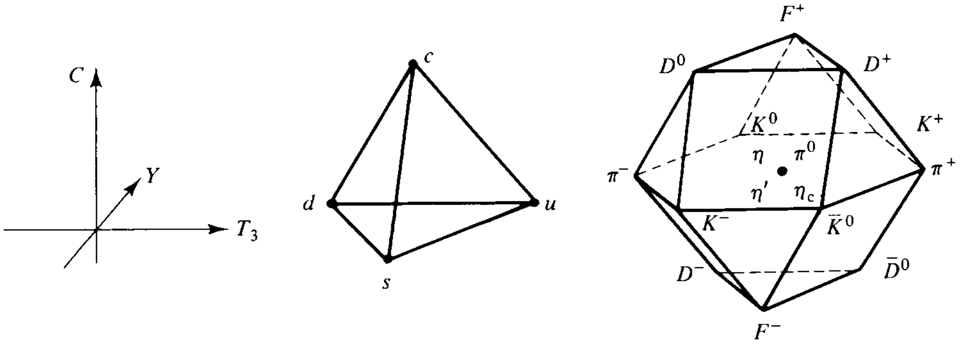


FIGURE 22.18 The four quarks u, d, s, c and their position in the three-dimensional weight space with the new quantum number "charm". By combining a quark and an antiquark one finds the 16 states on the right-hand side, of which 15 form an irreducible representation of SU(4). The new states D^0, D^+, F^+ and their antiparticles have been found in the laboratory.

22.6 Tensor Representations and Young Tableaux

A systematic construction of the tensor representation in direct product spaces such as $3 \times 3 \times 3$ is possible with the help of Young tableaux. The irreducible representation are obtained by forming tensors which are irreducible under permutations of the indices. They are of a definite symmetry type specified by the Young tableau introduced in App. 2A. The tableau $\boxed{1}\boxed{2}\boxed{3}$ indicates a tensor of complete symmetry transforming like a 10 representation, while $\begin{array}{c}\boxed{1}\\ \boxed{2}\\ \boxed{3}\end{array}$ corresponds to a complete antisymmetric tensor transforming like an SU(3) singlet. For the mixed tableau $\begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\end{array}$ we adopt the first convention to first symmetrize $|q_\alpha q_\beta q_\gamma\rangle$ in the first two indices, then antisymmetrize in the first and the third index. Equivalently we can use another tableaux, say $\begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\end{array}$ or $\begin{array}{ll}\boxed{2}&\boxed{1}\\ \boxed{3}&\end{array}$. Each gives an octet representation. For instance, the proton wave function (22.109) arises from the symmetry operations of the Young tableau $\begin{array}{ll}\boxed{2}&\boxed{1}\\ \boxed{3}&\end{array}$ applied to the state $|uud\rangle$. The symmetrization in the first two indices gives

$$|uud\rangle \rightarrow 2|uud\rangle \qquad \text{(symmetry in 21)}, \tag{22.139}$$

the antisymmetrization in the second and third index (of the original tensor $|q_\alpha q_\beta q_\gamma\rangle$)

$$|uud\rangle \rightarrow 2|u(ud-du)\rangle \qquad \text{(antisymmetry in 23)}. \tag{22.140}$$

Hence:

$$\begin{array}{ll}\boxed{2}&\boxed{1}\\ \boxed{3}&\end{array}\ |uud\rangle = 2|n(nd-du)\rangle = 2\sqrt{2}|p\rangle \tag{22.141}$$

Equivalent proton state could have been obtained from the tableaux

$$\begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\end{array}\ |uud\rangle = 2|uud-duu\rangle, \tag{22.142}$$

$$\begin{array}{ll}\boxed{1}&\boxed{2}\\ \boxed{3}&\end{array}\ |udu\rangle = 2|udu-duu\rangle, \tag{22.143}$$

or the sum of the two which gives

$$|u(ud+du)-2duu\rangle. \tag{22.144}$$

This is the proton state $|p'\rangle$ of Eq. (22.115) found in the product 6 × 3.
Which mixture of the two independent three-quark wave functions is verified by the proton in nature cannot be decided by SU(3) symmetry alone but must emerge from a dynamical model. We shall see later that the larger symmetry group SU(6) makes definite predictions.

In general, the dimensionality of the SU(n) representation of a tableaux is obtained from the following formula

$$d_{\text{SU}(n)} = \frac{D(l_1, l_2, \dots, l_n)}{D(n-1, n-2, \dots, 0)}, \tag{22.145}$$

where

$$D(x_1, \ldots, x_n) \equiv \prod_{i<j} (x_i - x_j), \tag{22.146}$$

and

$$l_i \equiv n + m_i - i, \qquad i = 1, 2, 3, \ldots, n, \tag{22.147}$$

with m_i being the number of boxes in the ith row of the tableau. Note that also rows with no boxes have to be counted, up to $i = n$.

A useful alternative formula for the dimension is

$$d_{\mathrm{SU}(n)} = \frac{l_1! l_2! \cdots l_n!}{0!1! \cdots (n-1)!} \frac{1}{\prod_{i,j} h_{ij}}, \tag{22.148}$$

where h_{ij} is the sum of the number of boxes to the right of the element ij in the tableau plus the number of boxes below ij plus 1.

Take some examples. The trivial Young tableau $\square$ has $m_1 = 1, m_2 = 0, m_3 = 0, \ldots, m_n = 0$ and thus $l_1 = n, l_2 = n - 2, \ldots, l_n = 0$. Hence

$$d_{\square} = n. \tag{22.149}$$

The first non-trivial one $\square\square$ has $m_1 = 2, m_2 = 0, \ldots, m_n = 0$ and thus $l_1 = n + 1, l_2 = n - 2, l_3 = n - 3, \ldots, l_n = 0$. Hence

$$d_{\square\square} = n(n+1)/2, \tag{22.150}$$

which for SU(3) gives 6. Further

$$d_{\begin{array}{c}\square\\ \square\end{array}} = n(n-1)/2, \tag{22.151}$$

which for SU(3) gives 3, the dimension of the representation $\bar{3}$.
For 3-quark states, the dimensions are

$$d_{\square\square\square} = n(n+1)(n+2)/6, \tag{22.152}$$

$$d_{\begin{array}{l}\square\square\\ \square\end{array}} = (n-1)n(n+1)/3, \tag{22.153}$$

$$d_{\begin{array}{c}\square\\ \square\\ \square\end{array}} = n(n-1)(n-2)/6, \tag{22.154}$$

which for SU(3) take the values 10, 8, 1, respectively. Somewhat more generally, the dimensions of some simple tableaux are

$$d_{\boxed{1}\boxed{2}\boxed{3}\cdots\boxed{k}} = \begin{pmatrix} n+k-1 \\ k \end{pmatrix}, \tag{22.155}$$

$$d_{\begin{array}{l}\boxed{1}\boxed{2}\boxed{3}\cdots\boxed{k}\\ \boxed{}\end{array}} = \binom{n+k-1}{k+1} k, \tag{22.156}$$

$$d_{\begin{array}{c}\boxed{1}\\ \boxed{2}\\ \vdots\\ \boxed{k}\end{array}} = \binom{n}{k}. \tag{22.157}$$

A column with n boxes is completely antisymmetric in the corresponding indices and thus proportional to the invariant antisymmetric tensor $\epsilon_{i_1 i_2,\dots,i_n}$. This is why its dimensionality is 1. In constructing all Young tableaux any such column can be omitted. For instance, in SU(3),

$$\begin{array}{l}\boxed{}\boxed{}\boxed{}\\ \boxed{}\boxed{}\\ \boxed{}\end{array} = \begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}. \tag{22.158}$$

One often indicates this cancellation by crossing out any complete column with a vertical line:

$$\begin{array}{l}\boxed{}\boxed{}\boxed{}\\ \boxed{}\boxed{}\\ \boxed{}\end{array} \rightarrow \begin{array}{l}\boxed{|}\boxed{}\boxed{}\\ \boxed{|}\boxed{}\\ \boxed{|}\end{array}. \tag{22.159}$$

The representation associated with each Young tableaux occurs as often as dimensionality of the associated representation of the permutation group. This follows from the fact that the representation matrices of the permutation group commute with those of SU(3). They can therefore be brought simultaneously to a block form along the diagonal

$$\begin{pmatrix} \boxed{D_1} & & & \\ & \boxed{D_1} & & \\ & & \boxed{\quad D_2 \quad} & \\ & & & \ddots \end{pmatrix}. \tag{22.160}$$

Along the diagonal there are n_i identical irreducible representation blocks D_i of dimensionality d_i, etc. Now, according to Schur's lemma, any matrix commuting with such a block matrix must be itself a block matrix with the dual form which consists of d_i identical blocks of dimensionality n_i. The formula for the dimensionality of the irreducible representations of the permutation group were given in App. 2A. If the Young tableau has r boxes the dimensionality is given by

$$d_{S_r} = \frac{r!}{\prod_{ij} h_{ij}}, \tag{22.161}$$

where the numbers h_{ij} are the same as in (22.145).

Using this formula we find, for instance, that the product of three-quark states $\square \times \square \times \square$ decompose into *one* SU(3) decuplet $\square\square\square$, *two* octets $\begin{array}{cc}\square&\square\\\square&\end{array}$, and *one* singlet $\begin{array}{c}\square\\\square\\\square\end{array}$:

$$3 \times 3 \times 3 = 10 + 8 + 8 + 1 \tag{22.162}$$

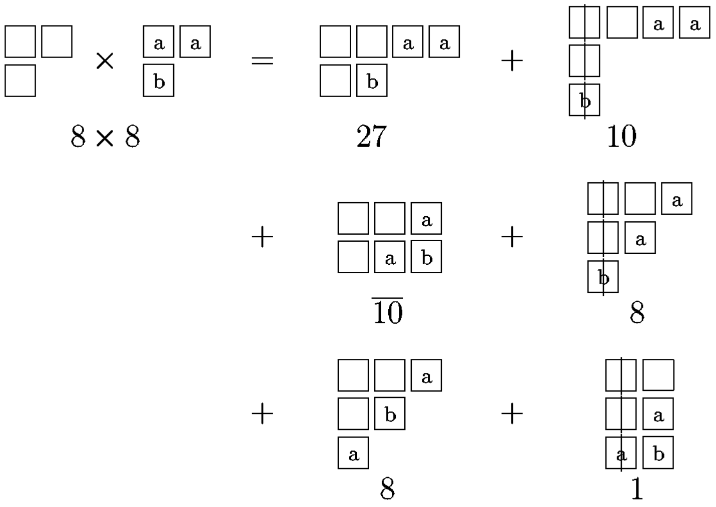
The Young tableau can also be used to find the irreducible contents in a product of two or more irreducible representations. For instance, suppose we want to know the irreducible contents of 8×8. We take the two Young tableaux $\begin{array}{cc}\square&\square\\\square&\end{array} \times \begin{array}{cc}\square&\square\\\square&\end{array}$ and distinguish the rows of boxes in the second factor by $a, b, c, \ldots$. In the example $\begin{array}{cc}\boxed{a}&\boxed{a}\\\boxed{b}&\end{array}$. Then we add the lettered boxes to the first tableau in the following way:

a) add all the a's, so as to get all proper tableaux (i.e. with $m_{i+1} \geq m_i$) which has no more than one a in each column.

b) add the b's once more in according to the same rule

c) add the c's … .

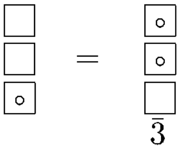
In this way we obtain in our example the expansion

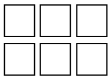


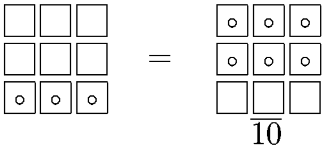
(22.163)

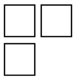
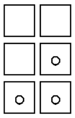
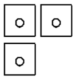
In accordance with the rule given earlier we have dropped all complete columns. Note that because of the antisymmetry of any complete column, an *incomplete* column is equivalent to the complex conjugate representation associated with the

Young tableau obtained from the missing boxes necessary to complete it (indicated ny a box with a circle), i.e.



This is how we can see immediately that the representation associated with the tableau  is a $\overline{10}$



The octet representation, being the adjoint representation of SU(3) , is real [its generators are $(G_a)_{bc} = -if_{abc}$ with real antisymmetric matrices $(f_a)_{bc}$; recall (3.79)]. From the Young tableau of the octet  this is obvious since the missing boxes in  form once more the same tableau , so the representation is equal to the complex conjugate of itself and thus real.

22.7 Effective Interactions among Hadrons

There exists a great variety of strongly interacting particles which many possible interactions between them. Let us study a few of them.

22.7.1 The Pion-Nucleon Interaction

The most important strong interaction is that between pions and nucleons since it provides for the dominant part of the forces which keep the nuclei together. If we neglect electromagnetic interactions, this interaction exhibits isospin symmetry pions nucleons, so that a system of and has the following effective action

$$\mathcal{A} = \mathcal{A}_\pi + \mathcal{A}_N + \mathcal{A}_{\pi NN} \tag{22.164}$$

$$\begin{aligned} \mathcal{A}_\pi &= \int d^4x \frac{1}{2} \left\{ [\partial \pi_a(x)]^2 - m_\pi^2 \pi_a^2(x) \right\} && (22.165)\\ \mathcal{A}_N &= \int d^4x \bar{N}(x)(i\partial\!\!\!/ - M_N)N(x) && (22.166)\\ \mathcal{A}_{\pi NN} &= \int d^4x g_{\pi NN} \bar{N}(x) i\gamma_5 \tau^a N(x) \pi_a(x) && (22.167) \end{aligned}$$

Here $\pi_a(x)$ is an isovector field and $N(x)$ a Dirac spinor field with an additional isospinor index which is not explicitly written down. The matrices τ^a are 2×2 Pauli matrices acting on the isospinor indices of $N(x)$. Studies of pion nucleon scattering amplitudes determine the size of the pseudoscalar coupling constant $g_{\pi NN}$ to be

$$\frac{g^2_{\pi NN}}{n\pi} \approx 14.4 \pm .4 \tag{22.168}$$

In some analyses, the pion nucleon interaction in (22.167) is parametrized in the axial vector form

$$\mathcal{A}_{\pi NN} = \frac{f_{\pi NN}}{M_\pi} \int d^4x \bar{N}(x) \gamma^\mu \gamma_5 \tau^a N(x) \partial_\mu \pi_a. \tag{22.169}$$

For physical nucleons on the mass shell, the two interactions are the same with the relation between the two coupling constants

$$f_{\pi NN} = -\frac{M_\pi}{2M_N} g. \tag{22.170}$$

Thus

$$f^2_{\pi NN} = 0.081 \pm 0.002. \tag{22.171}$$

In either form, the coupling strength is too large to perform perturbative calculations with the interaction $\mathcal{A}_{\pi NN}$.

It is useful to find the SU(3)-symmetric extension of the pion nucleon interaction. In SU(3), there are two ways of coupling three octets with each other, an antisymmetric one f_{ijk} a symmetric one, d_{ijk}. The easiest way to do calculation is by writing the nucleon octet as a 3×3 -matrix.

$$B = \begin{pmatrix} \frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda^0 & \Sigma^+ & p \\ \Sigma^- & -\frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda^0 & n \\ -\Xi^- & \Xi^0 & -\frac{2}{\sqrt{6}}\Lambda^0 \end{pmatrix} \tag{22.172}$$

and the pseudoscalar octet as

$$P = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta^0 & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta^0 & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta^0 \end{pmatrix}. \tag{22.173}$$

In this context the phases of $\pi^\pm$ are chosen as $\pi^\pm \equiv (\pi_1 \pm i\pi_2)/\sqrt{2}$ so that P is a hermitian matrix. Then the interaction Lagrangian has a simple explicit form

$$\mathcal{L}_{\text{PBB}} = g\frac{F}{F+D}\text{tr}\,([\bar{B}, B]P) + g\frac{D}{F+D}\text{tr}\,(\{\bar{B}, B\}P) \tag{22.174}$$

where $g \equiv g_{\pi NN}$ is the pion nucleon coupling constant and F/D the so called "F-over-D ratio", which gives the relative strength of antisymmetric and symmetric coupling. Working out the different components, this has the expansion in terms of isospinors

$$\begin{aligned}\mathcal{L}_{\rm int} &= g\Big\{(\bar{N}\boldsymbol{\tau}N)\cdot\boldsymbol{\pi}+(1-2\alpha)(\bar{\Xi}\boldsymbol{\tau}\Xi)\cdot\boldsymbol{\pi}+\frac{3-4\alpha}{\sqrt{3}}\bar{N}N\eta^0\\ &-\frac{3-2\alpha}{\sqrt{3}}\bar{\Xi}\Xi\eta^0-(1-2\alpha)(\bar{N}\boldsymbol{\tau}K)\cdot\boldsymbol{\Sigma}-(\bar{\Xi}\boldsymbol{\tau}K^c)\cdot\boldsymbol{\Sigma}\\ &-(1-2\alpha)\bar{\boldsymbol{\Sigma}}\cdot(K^\dagger\boldsymbol{\tau}N)-\bar{\boldsymbol{\Sigma}}\cdot(K^{c\dagger}\boldsymbol{\tau}\Xi)-\frac{3-2\alpha}{\sqrt{3}}\bar{N}\Lambda K\\ &-\frac{3-2\alpha}{\sqrt{3}}K^\dagger\bar{\Lambda}N+\frac{3-4\alpha}{\sqrt{3}}\bar{\Xi}\Lambda K^c+\frac{3-4\alpha}{\sqrt{3}}K^{c\dagger}\bar{\Lambda}\Xi\\ &+i(1-\alpha)(\bar{\boldsymbol{\Sigma}}\times\boldsymbol{\Sigma})\cdot\boldsymbol{\pi}+\frac{2\alpha}{\sqrt{3}}(\bar{\boldsymbol{\Sigma}}\Lambda)\cdot\boldsymbol{\pi}+\frac{2\alpha}{\sqrt{3}}(\bar{\Lambda}\boldsymbol{\Sigma})\cdot\boldsymbol{\pi}\\ &\qquad+\frac{2\alpha}{\sqrt{3}}(\bar{\boldsymbol{\Sigma}}\cdot\boldsymbol{\Sigma})\eta^0-\frac{2\alpha}{\sqrt{3}}\bar{\Lambda}\Lambda\eta^0\Big\}\end{aligned}\tag{22.175}$$

Here we have used the isospinors

$$N\equiv\begin{pmatrix}p\\ n\end{pmatrix},\quad \Xi\equiv\begin{pmatrix}\Xi^0\\ \Xi^-\end{pmatrix},\tag{22.176}$$

and

$$K\equiv\begin{pmatrix}K^+\\ K^0\end{pmatrix},\quad K^c\equiv\begin{pmatrix}\bar{K}^0\\ -K^-\end{pmatrix}.\tag{22.177}$$

Note that K^c is the charge conjugate spinor $C\bar{K}^*$. The parameter α is defined by

$$\alpha\equiv\frac{D}{F+D}\tag{22.178}$$

so that

$$F/D=(1-\alpha)/\alpha.\tag{22.179}$$

The two numbers $g=g_{\pi NN}$ and F/D parametrize all couplings.

The pion nucleon coupling was written down in Eq. (22.168). The F/D-ratio is determined experimentally from analysis of the production process

$$\pi^-p\rightarrow\Sigma^0K^+\tag{22.180}$$

which contains the coupling

$$\begin{aligned}g_{n\Sigma^-K^+} &\doteq -\sqrt{2}g(1-2\alpha)\\ &= -\sqrt{2}g\frac{F-D}{F+D}.\end{aligned}\tag{22.181}$$

From the experimental data one finds

$$\frac{F}{D}\approx\frac{2}{3}\tag{22.182}$$

For the coupling between pions and Σ-particles, the interaction Lagrangian (22.175) yields

$$g_{\Sigma\Sigma\pi} = g(1-\alpha) = g\frac{F}{F+D}, \tag{22.183}$$

The SU(3)-relations between coupling constants in the Lagrangian (22.175) are, of course, in agreement with standard SU(3) Clebsch-Gordan coefficients. The coefficients of the SU(2) subgroup can be taken from Table 3.2 in Chapter 3.1. The isoscalar factors form Table 22.4.

Take, for instance, the matrix element $\langle p|\pi^0|p\rangle$. The SU(2) Clebsch-Gordon coefficient is $1/\sqrt{3}$. The antisymmetric and symmetric isoscalar factors are $\sqrt{3}/\sqrt{12} = 1/2$ and $\sqrt{9}/\sqrt{20} = 3/2\sqrt{5}$, respectively. Hence, with the normalization factors of (22A.12),

$$\langle p|\pi^0|p\rangle = \frac{F+D}{2}. \tag{22.184}$$

The matrix element $\langle\Sigma^+|\pi^0|\Sigma^+\rangle$ has an SU(2) Clebsch-Gordan $1/\sqrt{2}$ and the isoscalar factors $\sqrt{2/3}$ and 0, respectively, so that

$$\langle\Sigma^+|\pi^0|\Sigma^+\rangle = F, \tag{22.185}$$

just before in (22.183).

Let us also calculate the coupling $g_{n\Sigma^-K^+}$ for which the Clebsch-Gordan coefficient is $-\sqrt{2/3}$ and the isoscalar factors are 1/2 and $-3/2\sqrt{5}$, respectively. Thus

$$\langle n|K^+|\Sigma^-\rangle = \frac{1}{\sqrt{2}}(F-D) \tag{22.186}$$

and

$$g_{n\Sigma^-K^+} = -\sqrt{2}\frac{F-D}{F+D} \tag{22.187}$$

as in (22.181).

22.7.2 The Decay $\Delta(1232) \to N\pi$

The interactions between the various members of the nucleon octet with pseudoscalar mesons and the decuplet resonances of spin-parity $J^P = 3/2^+$ are all determined by only a single SU(3)-invariant matrix element. This, in turn, may be chosen to coincide with the coupling between the proton, the π^+ and the $\Delta^{++}(1232)$ resonance. The Lagrangian for this specific interaction is conventionally written as

$$\mathcal{L}_{\Delta^{++}pn^+} = \frac{g^*}{M_N}\left(\bar{\psi}_\mu^{++}\psi^+\partial_\mu\pi^+ + \text{c.c.}\right) \tag{22.188}$$

where ψ_μ is a Rarita Schwinger spinor for the spin 3/2 particle $\Delta^{++}(1232)$. Some people write $4h/M_\pi$ instead of g^*/M_N.

The isospin structure can be incorporated by multiplying the Lagrangian by the Clebsch-Gordan factor

$$\frac{\langle\frac{3}{2}c|\frac{1}{2}a1b\rangle}{\langle\frac{3}{2}\frac{3}{2}|\frac{1}{2}\frac{1}{2}11\rangle} \tag{22.189}$$

where c, a, b are the isospin orientations of Δ, N and π. Alternatively, we can use Rarita Schwinger isospinors Δ_a (each of the three components $\Delta_1, \Delta_2, \Delta_3$ is a two-component isospinor) for the Δ particle and write in isospace (suppressing the Lorentz indices)

$$\mathcal{L} = \frac{g^*}{M_N}\left(\bar{\boldsymbol{\Delta}}N - \bar{N}\boldsymbol{\Delta}\right)\cdot\boldsymbol{\pi} \tag{22.190}$$

Indeed, the isospinor for the Δ^{++} resonance has only a +-component with isospin up so that $\bar{\boldsymbol{\Delta}}N\boldsymbol{\pi}$ contains the particles Δ^{++}, p, and π^+ in the form $\bar{\Delta}^{++}p\pi^+$ as in (22.188).

For calculations it is useful to record the completeness relation of Rarita-Schwinger isospinors

$$\sum_{s_3}\Delta_a\bar{\Delta}_b \;=\; \delta_{ab}\,1 - \frac{1}{3}\tau_a\tau_b = \frac{2}{3}\delta_{ab}\,1 - \frac{1}{6}[\tau_a, \tau_b], \tag{22.191}$$

where 1 stands for the 2×2 unit matrix in isospace.

The coupling g^* can be determined by an analysis of the strength of the Δ^{++} resonance in the π^+p scattering amplitude. This gives

$$g^* \approx 12.43 \approx 0.92 \tag{22.192}$$

corresponding to

$$h \approx 0.457 \tag{22.193}$$

If we assume the Δ resonance to be very narrow we can immediately calculate the decay rate from the interaction (22.188). The decay amplitude is found as follows. We consider a Δ^{++} resonance in its rest frame and use helicity amplitudes along the direction of the momentum of the emerging proton, which we assume to run in the 3-direction. The Δ helicity can be $\pm 3/2$ or $\pm 1/2$. Only the latter two orientations allow to conserve angular momentum with the helicities of the proton being $\pm 1/2$. The two orientations decay with the same rate, so we only need to study one case, say the helicity $+1/2$. The Rarita-Schwinger spinor is a Clebsch-Gordan combination of spin $J, M = 1, 0$ with $1/2, 1/2$ and of $J, M = 1, 1$ with $1/2 - 1/2$:

$$u_\mu(\mathbf{0}; \tfrac{3}{2}, \tfrac{1}{2}) = \sqrt{\frac{2}{3}}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} u(\mathbf{0}, \tfrac{1}{2}) + \frac{1}{\sqrt{6}}\begin{pmatrix} 0 \\ -1 \\ -i \\ 0 \end{pmatrix} u(\mathbf{0}, -\tfrac{1}{2}). \tag{22.194}$$

Between the state

$$a^\dagger_{\pi^+} a^\dagger_p |0\rangle \tag{22.195}$$

and a Δ state at rest $\langle 0|a_\Delta$ with unit normalization in a finite volume V, the wave functions are for the pion and the nucleon

$$\frac{1}{\sqrt{2E_\pi V}} e^{-iq_\pi x} \frac{1}{\sqrt{V}} u(p_N, s_3') \tag{22.196}$$

and for the Δ resonance

$$\frac{1}{\sqrt{V}} u_\mu(p_\Delta, s_3). \tag{22.197}$$

We therefore find the decay amplitude (the t-matrix)

$$\begin{aligned} t &= \frac{g^*}{M_N} \bar{u}_\mu u \, q^\mu \frac{1}{\sqrt{V}^3} \frac{1}{\sqrt{2E_\pi}} \frac{1}{\sqrt{E_N/M_N}} && (22.198) \\ &= \frac{g^*}{M_N} \sqrt{\frac{2}{3}} \cosh \frac{\zeta}{2} \, p_N \frac{1}{\sqrt{2E_\pi}} \frac{1}{\sqrt{V}^3} \frac{1}{\sqrt{E_N/M_N}}, && (22.199) \end{aligned}$$

where

$$u(p_N, \tfrac{1}{2}) u(0, \tfrac{1}{2}) = \cosh \frac{\zeta}{2} = \frac{1}{2M_N}(E_N + M_N) \tag{22.200}$$

with $E_N, E\pi$ being the energies of proton and pion in the rest frame of the decaying Δ resonance and p_N the momentum of the nucleon emerging in the z-direction. The decay rate is found from formula (7.239), for the helicity $h = 1/2$ state:

$$\begin{aligned} \Gamma_{\Delta^{h=1/2} \to N\pi} &= \frac{1}{(2\pi)^3} 2\pi \frac{E_N E_\pi}{M_\Delta} \int d\Omega |t|^2 \\ &= \frac{4\pi}{(2\pi)^3} 2\pi \frac{p_N}{M_\Delta} \frac{g^{*2}}{M_N^2} \frac{2}{3} p_N^2 \frac{1}{4} (E_N + M_N) \\ &= \frac{g^{*2}}{4\pi M_N^2} \frac{2}{3} \frac{p_N^3}{M_\Delta} (E_N + M_N). && (22.201) \end{aligned}$$

Since the Δ is with probability 1/2 in the helicity 3/2 state where it cannot decay, the final decay rate is only one half of (22.201), i.e.,

$$\Gamma = \frac{g^{*2}}{4\pi} \frac{1}{3} \frac{p_N^3}{M_\Delta} \left(\frac{E_N + M_N}{M_N^2} \right). \tag{22.202}$$

In terms of the three particle masses involved, the energy E_N is given by

$$E_N = \frac{{M_\Delta}^2 + M_N^2 - M_\pi^2}{2M_\Delta} \tag{22.203}$$

and the momentum p of the outcoming proton (and pion) by

$$p_N = \sqrt{[M_\Delta^2 - (M_N + M_\pi)^2][M_\Delta^2 - (M_N - M_\pi)^2]}/2M_\Delta. \tag{22.204}$$

Using the experimental width

$$\Gamma_\Delta \approx 115\text{MeV}, \tag{22.205}$$

we obtain

$$g^* \;\approx\; 14.43 \approx 1.07g \tag{22.206}$$

corresponding to

$$h \;\approx\; 0.53, \tag{22.207}$$

in reasonable agreement with independent determination (refx9.21), (22.193) from the pion nucleon scattering amplitudes.

It should be noted that the ratio $g^*/g \approx 1.07$ is a manifestation of SU(4) symmetry. Since the Δ resonance and the nucleon are in the same SU(4) multiplet 20 (corresponding to the SU(6) multiplet 56), all pion couplings are controlled by only one irreducible matrix element. In calculating them we have to take account of the fact that, in order to preserve parity, the pseudoscalar pion must emerge in a p wave. The matrix element between a Δ^+ resonance and a proton

$$\frac{1}{M_N}\bar{u}_\mu(\mathbf{0},\tfrac{1}{2})u(\mathbf{p}_N, s_3')iq_\pi^\mu \tag{22.208}$$

has for small momentum p_N in the z-direction the limiting form

$$-i\left[\sqrt{\frac{2}{3}}\frac{p_N}{M_N}\bar{u}(\mathbf{0},\tfrac{1}{2})u(\mathbf{0},\tfrac{1}{2}) + \frac{1}{\sqrt{6}M_N}(p_N^1 - ip_N^2)u(0,\tfrac{1}{2})\right]. \tag{22.209}$$

Thus it can be written in terms of two component spinors as

$$-2\sqrt{\frac{2}{3}}\frac{\mathbf{p}_N}{M_N}\chi(\tfrac{1}{2})\boldsymbol{\sigma}\chi(\tfrac{1}{2}). \tag{22.210}$$

The p-wave emission leads to the appearance of a spin matrix σ^i acting upon the helicity index of the nucleon. The same thing is observed for the matrix elements in the pseudoscalar pion nucleon coupling

$$\bar{u}(\mathbf{0},\tfrac{1}{2})i\gamma_5 u(\mathbf{p}_N,\tfrac{1}{2}). \tag{22.211}$$

For small momentum, this is given in

$$-i\,(\chi(\tfrac{1}{2}),\chi(\tfrac{1}{2}))\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\gamma_0\begin{pmatrix} e^{-\zeta\boldsymbol{\sigma}/2}\chi(\tfrac{1}{2}) \\ e^{\zeta\boldsymbol{\sigma}/2}\;\chi(\tfrac{1}{2}) \end{pmatrix} = -i\frac{\mathbf{p}_N}{M_N}\chi(\tfrac{1}{2})\boldsymbol{\sigma}\chi(\tfrac{1}{2}) \tag{22.212}$$

We now add the internal SU(2) structure and the SU(4)-matrix accompanying the emission of the pion in the z-direction of Δ^+ and the nucleon transforms like the tensor operator

$$\pi^a \hat{=} \tau^a \sigma^3. \tag{22.213}$$

The ratio of the couplings $p\pi^0 p$ and $\Delta^+\pi^0 p$ can therefore be found quite simply by applying $\tau^3\sigma^3$ to the proton state

$$\begin{aligned} p &= \frac{\sqrt{2}}{3}\Big[u^\uparrow u^\uparrow d^\downarrow + u^\uparrow u^\downarrow u^\uparrow + d^\downarrow u^\uparrow u^\uparrow \\ &\quad -\frac{1}{2}(u^\uparrow u^\downarrow d^\uparrow + u^\uparrow d^\uparrow u^\downarrow + u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + d^\uparrow u^\downarrow u^\uparrow)\Big], \end{aligned} \tag{22.214}$$

which gives

$$\begin{aligned} \tau^3\sigma^3 p &= \frac{\sqrt{2}}{3}\Big[3(u^\uparrow u^\uparrow d^\downarrow + u^\uparrow u^\downarrow u^\uparrow + d^\downarrow u^\uparrow u^\uparrow) \\ &\quad +\frac{1}{2}(u^\uparrow u^\downarrow d^\uparrow + u^\uparrow d^\uparrow u^\downarrow + u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + d^\uparrow u^\downarrow u^\uparrow)\Big]. \end{aligned} \tag{22.215}$$

This gives the matrix elements

$$\begin{aligned} p\tau^3\sigma^3 p &= \frac{2}{g}\left(3\cdot 3 - \frac{1}{4}\cdot 6\right) = \frac{5}{3}, \\ \Delta^+\tau^3\sigma^3 p &= \frac{\sqrt{2}}{g}\left(3\cdot 3 + \frac{1}{2}6\right) = \frac{4}{3}\sqrt{2}. \end{aligned} \tag{22.216}$$

For the ratio between g and g^* we have to go from $\Delta^+\tau^3\sigma^3 p$ to the matrix element $\Delta^{++}\tau^+\sigma^3 p$ which involves a Clebsch-Gordan factor

$$\Delta^{++}\tau^+\sigma^3 p = \frac{1}{\sqrt{2}}\frac{4}{3}\sqrt{2} = \frac{4}{3}. \tag{22.217}$$

Thus we obtain

$$\frac{g^*}{g} = \frac{4}{3}\frac{5}{3} = \frac{4}{5} = 0.8 \tag{22.218}$$

in reasonable agreement with the experimental ratio 0.92 from the analysis of pion nucleon scattering amplitudes.

By a similar quark calculation, we can predict from SU(6) symmetry the F/D ratio of the coupling between nucleon octets and pseudoscalar mesons. According to the interaction Lagrangian (22.175), the coupling $\Sigma^+\Sigma^+\pi^0$ is given by

$$g_{\Sigma^+\Sigma^+\pi^0} = g(1-\alpha) = g\frac{2F}{F+D}. \tag{22.219}$$

But this matrix element is easily calculated. The SU(6) state is obtained from $\Sigma^{+\uparrow}$ by applying V_- to it which changes the d quark into an s quark. Hence

$$\begin{aligned}\Sigma^{+\uparrow} = & -\frac{\sqrt{2}}{3}(u^\uparrow u^\uparrow s^\downarrow + u^\uparrow s^\downarrow u^\uparrow + s^\downarrow u^\uparrow u^\uparrow) \\ & -\frac{1}{2}\left(u^\uparrow u^\downarrow s^\uparrow + u^\uparrow s^\uparrow u^\downarrow + s^\uparrow u^\uparrow u^\downarrow + u^\downarrow u^\uparrow s^\uparrow + u^\downarrow s^\uparrow u^\uparrow + s^\uparrow u^\downarrow u^\uparrow\right).\end{aligned} \tag{22.220}$$

Applying $\tau_3\sigma_3$ gives

$$\tau_3\sigma_3\Sigma^{+\uparrow} = -\frac{\sqrt{2}}{3}\,2(u^\uparrow u^\uparrow s^\downarrow + u^\uparrow s^\downarrow u^\uparrow + s^\downarrow u^\uparrow u^\uparrow). \tag{22.221}$$

The scalar product with $\Sigma^{+\uparrow}$ gives

$$\Sigma^{+\uparrow}\tau_3\sigma_3\Sigma^{+\uparrow} = \frac{4}{3}. \tag{22.222}$$

In comparison with the pion nucleon matrix element $g_{\pi NN} = g$, this amounts to the relation

$$g_{\pi^0\Sigma^+\Sigma^+} = \frac{4}{5}g. \tag{22.223}$$

We therefore find the F/D ratio the SU(6) value

$$F/D = 2/3. \tag{22.224}$$

in good agreement with the experimental determination. In App. A we have collected a few useful formulas for the SU(3) calculations involved.

22.7.3 The Vector Meson Decay $\rho(770) \rightarrow \pi\pi$

Among mesons, the most directly observable coupling is the $\rho\pi\pi$ coupling. It governs the strength of the most prominent resonance in the $S(770)$ pion pion scattering amplitude. Since ρ is a vector meson of isospin 1 it is coupled to the two pions in a p- wave. The Lagrangian interaction is given by

$$\mathcal{L} = \frac{g_{\rho\pi\pi}}{2}\boldsymbol{\rho}^\mu \cdot \left(\boldsymbol{\pi}\times \overleftrightarrow{\partial}_\mu\, \boldsymbol{\pi}\right) \tag{22.225}$$

For the decay $\rho^+ \rightarrow \pi^0\pi^-$, the invariant matrix element t is given by

$$\langle\pi^0\pi^+|t|\rho^+\rangle = -g_{\rho\pi\pi}\frac{1}{\sqrt{2VE_{pi}}^2}\frac{1}{\sqrt{2VM_\rho}}2p_\pi^\mu\epsilon_\mu(p_\rho, s_3) \tag{22.226}$$

where $\epsilon_\mu(p_\rho, s_3)$ is the polarization vector of the ρ meson and the decay rate is, according to formula ( ),

$$\Gamma = g_{\rho\pi\pi}^2\frac{4\pi}{(2\pi)^2}\frac{p_{\rm CM}}{M_\rho^2}\frac{1}{2^3}4|p_\pi^\mu\epsilon_\mu|^2. \tag{22.227}$$

The average over the initial polarization gives

$$\frac{1}{3}p_\pi^\mu p_\pi^\nu \sum_{s_3} \epsilon^\mu(p_\rho, s_3)\epsilon^\nu(p_\rho, s_3) = -\frac{1}{3}p_\pi^\mu p_\pi^\nu \left(g_{\mu\nu} - \frac{p_\rho^\mu p_\rho^\nu}{p_\rho^2}\right) = \frac{1}{3}\mathbf{p}_\pi^2. \tag{22.228}$$

Hence

$$\begin{aligned} \Gamma_{\rho^+\to\pi^0\pi^+} &= \frac{g_{\rho\pi\pi}^2}{4\pi}\frac{2}{3}\frac{\mathbf{p}_\pi^3}{M_\rho^2} \\ &= \frac{g_{\rho\pi\pi}^2}{4\pi}\frac{2}{3}\frac{\left(M_\rho^2 - 4m_\pi^2\right)^{3/2}}{8M_\rho^2}. \end{aligned} \tag{22.229}$$

The experimental decay width is

$$\Gamma_{\rho\pi\pi} \approx 153\text{MeV}. \tag{22.230}$$

From this one finds the coupling constant

$$\frac{g_{\rho\pi\pi}^2}{4\pi} \approx 2.85. \tag{22.231}$$

Another important coupling is that between ω, ρ, and π:

$$\mathcal{L}_{\omega\rho\pi} = g_{\omega\rho\pi}\epsilon_{\mu\nu\lambda\kappa}\partial^\mu\omega^\nu\partial^\lambda\boldsymbol{\rho}^\kappa \cdot \boldsymbol{\pi}. \tag{22.232}$$

It is responsible for the decay

$$\omega \longrightarrow \pi\pi\pi \tag{22.233}$$

which proceeds at a rate

$$\Gamma_{\omega\to\pi\pi\pi} = 9.8 \pm .3\, MeV \tag{22.234}$$

The $\pi\pi$ channels are dominated by the ρ resonance. One can therefore assume a sequential decay and finds that

$$\begin{aligned} \Gamma_{\omega\to 3\pi} &= (M_\omega - 3M_\pi)^4 \left(M_\rho^2 - 4M_\pi^2\right)^{-2} M_\omega M_\pi^2 \frac{1}{\sqrt{27}}\frac{1}{4}\frac{g_{\rho\pi\pi^2}}{4\pi}\frac{g_{\omega\rho^2\pi}}{4\pi} \times 3.56 \\ &\approx 10.3\text{MeV}\frac{{g_{\rho\pi}}^2}{4\pi}\frac{{g_{a\rho\pi}}^2}{4\pi} \end{aligned} \tag{22.235}$$

where the number 3.56 is due to the numeric integration of a phase space integral[7]. The experimental rate gives

$$\frac{g_{\rho\pi\pi}^2}{4\pi}\frac{g_{\rho\pi\pi}^2}{4\pi} \approx \frac{0.95}{M_\pi^2} \tag{22.236}$$

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[7] For details see M. Gell-Mann, D. Sharp, W.G. Wagner, Phys. Rev. Lett. *8*, 261 (1962)

and hence

$$\frac{g_{\omega\rho\pi}^2}{g_{\rho\pi\pi}{}^2} \approx \frac{0.117}{M_\pi^2} \approx 6.14(\mathrm{GeV})^{-2}. \tag{22.237}$$

In πK scattering one observes the SU(3) partner of the ρ meson, the strange vector meson K^* (892). Its coupling is written as

$$\mathcal{L} = \frac{1}{2} g_{K^*K\pi}(K^\dagger \boldsymbol{\tau} K) i\overleftrightarrow{\partial}_\mu \boldsymbol{\pi}. \tag{22.238}$$

Its decay width is

$$\Gamma_{K^*\pi\pi} = 3\frac{\left(\frac{1}{2}g_{K^*K\pi}\right)^2}{4\pi}\frac{2}{3}\frac{p_{\mathrm{CM}}^3}{M_K^2} \tag{22.239}$$

with

$$p_{\mathrm{CM}} = \frac{1}{2M_{K^*}}\sqrt{\left[M_{K^*}^2 - (M_{K^*} + M_\pi)^2\right]\left[M_{K^*}^2 - (M_{K^*} - M_\pi)^2\right]}. \tag{22.240}$$

Thus the ratio with respect to the $\rho\pi\pi$ width is

$$\begin{aligned} \frac{\Gamma_{K^*K\pi}}{\Gamma_{\rho\pi\pi}} &= \frac{3}{4}\frac{g_{K^*K\pi}^2}{g_{\rho\pi\pi}^2}\frac{M_\rho^2}{M_{K^*}^2}\frac{p_{\mathrm{CM}\,K^*}^3}{p_{\mathrm{CM}\,\rho}^3} \\ &\approx \frac{3}{4}\frac{g_{K^*K\pi}^2}{g_{\rho\pi\pi}^2} \times 0.385. \end{aligned} \tag{22.241}$$

With the experimental value

$$\Gamma_{K^*K\pi} = (51.8 \pm 0.8)\mathrm{MeV} \tag{22.242}$$

the experimental width ratio is 0.3406 and hence

$$\frac{p_{\mathrm{CM}\,K^*}}{p_{\mathrm{CM}\,\rho}} \approx 1.086. \tag{22.243}$$

Note that by SU(3) symmetry this ratio should be unity, which it is to a good approximation.

22.7.4 The Axial Vector Meson Decay $a_1(1270) \to \rho\pi$

A more involved coupling governs the decay of the axial vector meson $a_1(1270)$. It is seen as a resonance of width

$$\Gamma_{a,\rho\pi} \approx 316 \pm 45\mathrm{MeV} \tag{22.244}$$

is the $\rho - \pi$ scattering amplitude. Angular momentum and parity allow for s- and d-wave interactions so that there exist two independent coupling constants with a Lagrangian density

$$\mathcal{L} = g_{a_1\rho\pi}\left(\mathbf{a}_\mu \times \boldsymbol{\rho}^\mu\right) \cdot \boldsymbol{\pi} + h_{a_1\rho\pi}\left(\partial_\mu \mathbf{a}^\nu \times \partial_\nu \boldsymbol{\rho}^\mu\right) \cdot \boldsymbol{\pi} \tag{22.245}$$

If $\epsilon(p), \epsilon(q)$ denote the polarization vectors of the a_1 and ρ meson, respectively, and k the momentum of the outgoing pion, the invariant matrix element for $A^+ \longrightarrow \rho^- \pi^+$ reads

$$t_{ba} = \frac{1}{\sqrt{2V}^3} \frac{1}{\sqrt{p_0 q_0 k_0}} \left[g_{a_1\rho\pi} \epsilon^*_\mu(p) \epsilon^\mu(q) - h_{a_1\rho\pi} q_\nu \epsilon^{*\nu}(p) p^\mu \epsilon_\mu(q)\right] \tag{22.246}$$

For the calculation of decay rates it is better to use a more complicated looking decomposition into a longitudinal and a transverse helicity amplitude

$$\begin{aligned} t^L &= \frac{1}{\sqrt{2V}^3} \frac{1}{\sqrt{p_0 q_0 k_0}} g_L P_\mu q^\nu \left(g_{\mu\lambda} - \frac{q_\mu q_\lambda}{q^2}\right) \left(g_{\nu\kappa} - \frac{p_\nu p_\kappa}{p^2}\right) \epsilon^* * \kappa(p) \epsilon^\lambda(q) \\ t^T &= -\frac{g_T}{m_a^2} \epsilon^{\mu\alpha'\beta'}{}_\gamma \epsilon^{\lambda\alpha\beta\gamma} q_\beta p_\alpha q_{\beta'} p_{\alpha'} \epsilon^*_\lambda(p) \epsilon_\mu(q) \end{aligned} \tag{22.247}$$

The relation between the two is

$$\begin{aligned} -h_{a_1\rho\pi} &= g_L + g_T \frac{m_{a_1}^2 + m_\rho^2 - m_\pi^2}{2m_{a_1}^2} \\ -g_{a_1\rho\pi} &= \frac{g_T}{m_{a_1}^2} \left[\left(\frac{m_{a_1}^2 + m_\rho^2 - m_\pi^2}{2}\right)^2 - m_{a_1}^2 m_\rho^2\right] \end{aligned} \tag{22.248}$$

The advantage of these amplitude is that they decouple in the decay process. A somewhat tedious calculation (see Appendix 22B) gives

$$\Gamma_{a_1\rho\pi} = \Gamma^L_{a_1\rho\pi} + \Gamma^T_{a_1\rho\pi} \tag{22.249}$$

with

$$\begin{aligned} \Gamma^L_{a_1\rho\pi} &= \frac{g_L^2}{n\pi} \frac{1}{3} \frac{p_\rho^5}{m_\rho^2} \\ \Gamma^T_{a_1\rho\pi} &= \frac{g_T^2}{n\pi} \frac{2}{3} \frac{p_\rho^5}{m_{a_1}^2} \end{aligned} \tag{22.250}$$

with the experimental masses having the ratio

$$\frac{m_{a_1}^2}{m_\rho^2} \approx 2.72 \tag{22.251}$$

we can write

$$\Gamma_{a_1\rho\pi} \approx 5.5 \times 10^{-5} \left(g_L^2 + 2.735\, g_T^2\right) \mathrm{GeV} \tag{22.252}$$

and find for the coupling constants the relation

$$g_L^2 + \frac{2m_\rho^2}{m_{a_1}^2} g_T^2 \approx g_L^2 + 0.68 g_T^2 \approx 75.1 \tag{22.253}$$

The ration between the two coupling constants has to be determined by some other method.

Appendix 22A Useful SU(3) Formulas

The matrix elements of an octet operator between two octets labeled by the real indices $i = 1, 2, 3, \ldots, 8$ of the adjoint representation 8 can be written as follows

$$\langle 8_i | 8_k 8_j \rangle = F(-i f_{kij}) + D d_{kij} = F(\hat{F}_k)_{ij} + D(\hat{D}_k)_{ij} \tag{22A.1}$$

where f_{ijk} are the structure constants of SU(3) and d_{ijk} those of the anticommutators

$$\{\lambda_i, \lambda_j\} = d_{ijk}\lambda_k + \frac{4}{3}\delta_{ij}.$$

The SU(3) vector e^i associated with a specific particle is found from the assignment of the nucleon octet to the 3×3 -matrix elements

$$N = \begin{pmatrix} \frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda & \Sigma^+ & p \\ \Sigma^- & -\frac{1}{\sqrt{2}}\Sigma^0 + \frac{1}{\sqrt{6}}\Lambda & n \\ \Xi^- & \Xi^0 & -\frac{1}{\sqrt{6}}2\Lambda \end{pmatrix}. \tag{22A.2}$$

By contraction this with the λ-matrices and forming

$$e^i = \frac{1}{\sqrt{2}} \mathrm{tr}\left(\lambda^i N\right). \tag{22A.3}$$

The proton, for example, corresponds to the octet vector

$$e^i(p) = \frac{1}{\sqrt{2}} \mathrm{tr}\left[\lambda^i \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]. \tag{22A.4}$$

It has the non-zero components

$$e^4(p) = \frac{1}{\sqrt{2}}, \quad e^5(p) = \frac{i}{\sqrt{2}}. \tag{22A.5}$$

For the π^0 couplings we calculate the matrix elements $\hat{F}_{0ij}\hat{D}_{0ij}$ between two proton states as follows: This gives

$$\langle p|\hat{F}_0|p\rangle = \frac{1}{2}, \quad \langle p|\hat{D}_0|p\rangle = \frac{1}{2}. \tag{22A.6}$$

Hence

$$\langle p|\pi_0|p\rangle = \frac{F+D}{2}. \tag{22A.7}$$

Similarly, the SU(3) vector of the Σ^+ particle is

$$e^i(\Sigma^+) = \frac{1}{\sqrt{2}}\mathrm{tr}\left[\lambda^i\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]. \tag{22A.8}$$

It has the non-zero components

$$\begin{aligned} e^1\left(\Sigma^+\right) &= \frac{1}{\sqrt{2}} \\ e^2\left(\Sigma^+\right) &= \frac{i}{\sqrt{2}}. \end{aligned} \tag{22A.9}$$

The coupling of π^0 to Σ particles we need the matrix elements $(\hat{F}_0)_{ij}$, $(\hat{D}_0)_{ij}$ between Σ^+ states and find

$$\begin{aligned} \langle\Sigma^+|\hat{F}_0|\Sigma^+\rangle &= 1 \\ \langle\Sigma^+|\hat{D}_0|\Sigma^+\rangle &= 0. \end{aligned} \tag{22A.10}$$

Hence

$$\langle\Sigma^+|\pi^0|\Sigma^+\rangle = F. \tag{22A.11}$$

The matrix elements of π^+ between $\Sigma\Sigma$ and pp have therefore the ratio

$$\frac{\Sigma^+\pi^+\Sigma^+}{p\pi p} = \frac{2F}{F+D}$$

just as in (22.183), (22.185), and (22.219).

Another way to calculate SU(3)-matrix elements makes use of tables of the SU(3) Clebsch-Gordan coefficients. The matrices $\hat{F}_i$ $\hat{D}_i$ correspond to the coefficients

$$\hat{F}_i = \sqrt{3}\langle 8_a|88\rangle, \qquad \hat{D}_i = \sqrt{\frac{5}{3}}\langle 8_s|8\,8\rangle. \tag{22A.12}$$

The Clebsch Gordan coefficients can be decomposed into a product of an isospin SU(2) Clebsch Gordan coefficients and a so-called isoscalar factor

$$\langle 8_a i|8j;8k\rangle = \langle\langle 8_a Y_i|8Y_j;8Y_k\rangle\rangle(T^i,T_3^i|T^j,T_3^j;T^k,T_3^k), \tag{22A.13}$$

where T^i, T_3^i is the isospin contents of the SU(3) index i. The isoscalar factors are listed in Table 22.4.

TABLE 22.4 Isoscalar Factors of SU(3)

$\mathbf{1} \to \mathbf{8} \otimes \mathbf{8}$

$$(\Lambda) \to (N\bar K\ \Sigma\pi\ \Lambda\eta\ \Xi K) = \frac{1}{\sqrt{8}} \begin{pmatrix} 2\ 3\ -1\ -2 \end{pmatrix}^{1/2}$$

$\mathbf{8}_1 \to \mathbf{8} \otimes \mathbf{8}$

$$\begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Sigma \end{pmatrix} \to \begin{pmatrix} N\pi\ N\eta\ \Sigma K\ \Lambda K \\ N\bar K\ \Sigma\pi\ \Lambda\pi\ \Sigma\eta\ \Xi K \\ N\bar K\ \Sigma\pi\ \Lambda\eta\ \Xi K \\ \Sigma\bar K\ \Lambda\bar K\ \Xi\pi\ \Xi\eta \end{pmatrix} = \frac{1}{\sqrt{20}} \begin{pmatrix} 9\ -1\ -9\ -1 \\ -6\ 0\ 4\ 4\ -6 \\ 2\ -12\ -4\ -2 \\ 9\ -1\ -9\ -1 \end{pmatrix}^{1/2}$$

$\mathbf{8}_3 \to \mathbf{8} \otimes \mathbf{8}$

$$\begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix} \to \begin{pmatrix} N\pi\ N\eta\ \Sigma K\ \Lambda K \\ N\bar K\ \Sigma\pi\ \Lambda\pi\ \Sigma\eta\ \Xi K \\ N\bar K\ \Sigma\pi\ \Lambda\eta\ \Xi K \\ \Sigma\bar K\ \Lambda\bar K\ \Xi\pi\ \Xi\eta \end{pmatrix} = \frac{1}{\sqrt{12}} \begin{pmatrix} 3\ 3\ 3\ -3 \\ 2\ 8\ 0\ 0\ -2 \\ 6\ 0\ 0\ 6 \\ 3\ 3\ 3\ -3 \end{pmatrix}^{1/2}$$

$\mathbf{10} \to \mathbf{8} \otimes \mathbf{8}$

$$\begin{pmatrix} \Delta \\ \Sigma \\ \Xi \\ \Omega \end{pmatrix} \to \begin{pmatrix} N\pi\ N\eta \\ N\bar K\ \Sigma\pi\ \Lambda\pi\ \Sigma\eta\ \Xi K \\ \Sigma\bar K\ \Lambda\bar K\ \Xi\pi\ \Xi\eta \\ \Xi\bar K \end{pmatrix} = \frac{1}{\sqrt{12}} \begin{pmatrix} -6\ 6 \\ -2\ 2\ -3\ 3\ 3 \\ 3\ -3\ 3\ 3 \\ 12 \end{pmatrix}^{1/2}$$

$\mathbf{8} \to \mathbf{10} \otimes \mathbf{8}$

$$\begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix} \to \begin{pmatrix} \Delta\pi\ \Sigma K \\ \Delta\bar K\ \Sigma\pi\ \Sigma\eta\ \Xi K \\ \Sigma\pi\ \Xi K \\ \Sigma\bar K\ \Xi\pi\ \Xi\eta\ \Omega K \end{pmatrix} = \frac{1}{\sqrt{15}} \begin{pmatrix} -12\ 3 \\ 8\ -2\ -3\ 2 \\ -9\ 6 \\ 3\ -3\ -3\ 6 \end{pmatrix}^{1/2}$$

$\mathbf{10} \to \mathbf{10} \otimes \mathbf{8}$

$$\begin{pmatrix} \Delta \\ \Sigma \\ \Xi \\ \Omega \end{pmatrix} \to \begin{pmatrix} \Delta\pi\ \Delta\pi\ \Sigma K \\ \Delta\bar K\ \Sigma\pi\ \Sigma\eta\ \Xi K \\ \Sigma\bar K\ \Xi\pi\ \Xi\eta\ \Omega K \\ \Xi\ \bar K\Omega\eta \end{pmatrix} = \frac{1}{\sqrt{24}} \begin{pmatrix} 15\ 3\ -6 \\ 8\ 8\ 0\ -8 \\ 12\ 3\ -3\ -6 \\ 12\ -12 \end{pmatrix}^{1/2}$$

Appendix 22B Decay rate for $a_1 \to \rho\pi$

Denoting the polarization tensors of the a_1 and ρ mesons $\epsilon(p)$ by ϵ', $\epsilon(q)$ by ϵ, and using the transversality properties $p_\mu \epsilon' = 0$, $q_\mu \epsilon^\mu = 0$, respectively, the amplitudes are (dropping the normalization factors $1/\sqrt{2Nq_0}$ associated with the three particles)

$$\begin{aligned} t &= g_L(p\epsilon'^*)(q\epsilon) + \frac{g_T}{M_{a_1}^2} \begin{vmatrix} \epsilon'^*\epsilon & \epsilon'^*q & \epsilon'^*p \\ \epsilon q & q^2 & qp \\ \epsilon p & qp & p^2 \end{vmatrix} \\ &= g_L(p\epsilon')(q\epsilon) + \frac{g_T}{M_{a_1}^2}\left[M_{a_1}^2 M_\rho^2(\epsilon'^*\epsilon) + (p\epsilon'^*)qp - (\epsilon'^*\epsilon)(qp)^2\right]. \end{aligned} \tag{22B.1}$$

This expression shows directly the relation of the couplings g_L and g_T with the couplings $g_{a_1,\rho\pi}$ and $h_{a_1\rho\pi}$. We now put a_1 in its rest frame so that $p = (M_{a_1}000)$ and have the scalar products

$$\begin{aligned} \epsilon'^*(q, \substack{1\\2})\epsilon^*(p, \substack{1\\2}) &= -1 \\ \epsilon'^*(q,3)\epsilon(p,3) &= -\frac{q_0}{M_\rho} \end{aligned}$$

$$\begin{aligned} &(q\epsilon(p, \substack{1\\2})) = 0 \qquad (p\epsilon'^*(q, \substack{1\\2})) = 0, \\ &(q\epsilon(p,3)) = -p_{\mathrm{CM}}, \qquad (p\epsilon'^*(q,3)) = \frac{p_{\mathrm{CM}}}{M_\rho} M_{a_1}, \end{aligned} \tag{22B.2}$$

where

$$p_{\mathrm{CM}} = \frac{1}{2M_{a_1}}\sqrt{[M_{a_1}^2 - (M_\rho - M_\pi)^2][M_{a_1^2} - (M_\rho - M_\pi)^2]} \tag{22B.3}$$

is the center-of-mass momentum of the ρ-meson. We therefore find the helicity amplitudes (writing the helicities as superscripts in parentheses)

$$\begin{aligned} \langle \rho^{(0)}\pi_1|t|a_1(0)\rangle &= -g_L p_{\mathrm{CM}}^2 \frac{M_{a_1}}{M_\rho} \\ \langle \rho^{\substack{1\\2}}\pi|t|a_1^{\substack{1\\2}}\rangle &= \frac{g_T}{M_{a_1}^2}\left(-M_{a_1}^2 M_\rho^2 + E_{\mathrm{CM}}^2 M_{a_1}^2\right) = g_T p_{\mathrm{CM}}^2, \end{aligned} \tag{22B.4}$$

where

$$E_{\mathrm{CM}} = \frac{M_{a_1}^2 + M_\rho^2 - M_\pi^2}{2M_{a_1}} \tag{22B.5}$$

is the energy of the ρ meson in the center-of-mass frame. From this we obtain directly the longitudinal width

$$\Gamma^L_{a_1\to\rho\pi} = \frac{g_L^2}{4\pi}\frac{2}{6}\frac{p_{\mathrm{CM}}^5}{M_\rho^2}, \tag{22B.6}$$

having inserted a factor 2 due to isospin, and a transversal width

$$\Gamma^T_{a_1\to\rho\pi} = \frac{g_T^2}{4\pi}\frac{2}{6}\cdot 2\frac{p_{\rm CM}^5}{M_{a_1}^2} \tag{22B.7}$$

$$\begin{aligned} \begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix}_{8_s} &\rightarrow \left(\begin{array}{c} N\pi \;\; N\eta \;\; \Sigma K \;\; \Lambda K \\ N\bar{K} \;\; \Sigma\pi \;\; \Lambda\pi \;\; \Sigma\eta \;\; \Xi K \\ N\bar{K} \;\; \Sigma\pi \;\; \Lambda\eta \;\; \Xi K \\ \Sigma K \;\; \Lambda\bar{K} \;\; \Xi\pi \;\; \Xi\eta \end{array}\right) \\ &= \frac{1}{\sqrt{20}}\left(\begin{array}{c} 3 \;\; -1 \;\; -3 \;\; -1 \\ -\sqrt{6} \;\; 0 \;\; 2 \;\; 2-\sqrt{6} \\ \sqrt{2} \;\; -\sqrt{12} \;\; -2 \;\; -\sqrt{2} \\ 3 \;\; -1 \;\; -3 \;\; -1 \end{array}\right) \end{aligned} \tag{22B.8}$$

while the antisymmetric coupling is

$$\begin{aligned} \begin{pmatrix} N \\ \Sigma \\ \Lambda \\ \Xi \end{pmatrix}_{8_a} &\rightarrow \left(\begin{array}{c} N\pi \;\; N\eta \;\; \Sigma K \;\; \Lambda K \\ N\bar{K} \;\; \Sigma\pi \;\; \Lambda\pi \;\; \Sigma\eta \;\; \Xi K \\ N\bar{K} \;\; \Sigma\pi \;\; \Lambda\eta \;\; \Xi K \\ \Sigma\bar{K} \;\; \Lambda\bar{K} \;\; \Xi\pi \;\; \Xi\eta \end{array}\right) \\ &= \frac{1}{\sqrt{12}}\left(\begin{array}{c} \sqrt{3} \;\; \sqrt{3} \;\; \sqrt{3} \;\; \sqrt{3} \\ \sqrt{2} \;\; \sqrt{8} \;\; 0 \;\; -\sqrt{2} \\ \sqrt{6} \;\; 0 \;\; 0 \;\; 6 \\ \sqrt{3} \;\; \sqrt{3} \;\; \sqrt{3} \;\; -\sqrt{3} \end{array}\right). \end{aligned} \tag{22B.9}$$

23

Symmetries Linking Internal and Spacetime Structure. Supersymmetry

Besides space-time symmetries under the Lorentz and Poincarè group and approximate internal symmetries under SU(2), SU(3), etc., there exists a further class of approximate symmetries which combine external and internal indices. Historically, the first example for this class of symmetries arose in nuclear physics where isospin was combined with spin to form the larger group SU(4).

23.1 Approximate SU(4)-Symmetry of Nuclear Forces

Soon after the discover of the approximate isospin symmetry in nuclear physics, the search went on for even higher approximate symmetries. It turned out that the nuclear forces had also an approximate independence of spin. Moreover, this could be combined with isospin to form an approximate invariance under the larger group SU(4). The different terms in the potential between nucleons are conventionally classified by their behavior under certain interchange operators acting upon two-nucleon wave functions. These are defined as follows:

$$\begin{aligned} P^M\psi(x_1a_1,x_2a_2) &\equiv \psi(x_2a_1,x_1a_2) \text{ Majorana Operator,} \\ P^B\psi(x_1a_1,x_2a_2) &\equiv \psi(x_1a_2,x_2a_1) \text{ Bartlett Operator,} \\ P^H\psi(x_1a_1,x_2a_2) &\equiv \psi(x_2a_2,x_1a_1) \text{ Heisenberg Operator,} \end{aligned} \tag{23.1}$$

where x denotes the positions and a the third components of spin, s_3, of the particles. The effect of the interchange operators on two-nucleon wave functions of definite orbital angular momentum l and spin (singlet or triplet) is shown in Table 23.1. Using these operators, the most general two-particle potential can be written as follows

$$\begin{aligned} V = V_W(r) + V_M(r)P^M + V_B(r)P^B + V_H(r)P^H \\ +V_{TW}(r)S_{12} + V_{TM}(r)S_{12}P^M, \end{aligned} \tag{23.2}$$

where S_{12} is the spin orbit coupling operator

$$S_{12} \equiv 3(\boldsymbol{\sigma}_1\hat{\mathbf{r}})(\boldsymbol{\sigma}_2\hat{\mathbf{r}}) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2). \tag{23.3}$$

TABLE 23.1 Action of the different interchange operators.

	even l		odd l	
	triplet	singlet	triplet	singlet
P^M	1	1	-1	-1
P^B	1	-1	1	-1
P^H	1	-1	-1	1

Here $\hat{\mathbf{r}} \equiv \mathbf{r}/|\mathbf{r}|$ is the direction of the distance vector $\mathbf{r}$ between the two particles. The $\boldsymbol{\sigma}$-matrices $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ act on the spin indices of the particles 1, 2, respectively. This is, in fact, the most general way of describing noncentral forces which can be derived from a potential. The potential $\omega(\sigma)$ is called *Wigner potential* and is purely central. The potential V_{TW} proportional to the operator S_{12} provides for the so-called *tensor force* which is responsible for mixing the ${}^3_1D$ wave into the ${}^3_1S$ ground state wave function[1] of the deuteron ($\approx 2-6\,\%$). Note that in a spin singlet states $S_{12}=0$. The potential V_M is called *Majorana potential.* The Bartlett operator P_B can be expressed in terms of the Pauli spin matrices as follows

$$P^B = \frac{1}{2}(1+\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2). \tag{23.4}$$

In this parametrization, each of the six V-terms is proportional to the unit matrix in the space of charge indices.

Let us define, in this space, the operator

$$P^\tau \equiv \frac{1}{2}(1+\boldsymbol{\tau}_1\boldsymbol{\tau}_2), \tag{23.5}$$

where $\boldsymbol{\tau}$ denotes a three-component vector of Pauli matrices, $\boldsymbol{\tau}=(\tau^1,\tau^2,\tau^3)$, which, instead of spin, act on the isospin indices of the nucleons. It is easy to verify that $P^H=-P^\tau$ for wave functions which satisfy the Pauli principle and that

$$P^M = P^B P^H. \tag{23.6}$$

The action of the spin isospin operators is shown in Table 23.2. It is then possible to rewrite the potential (23.1) in terms of the $\boldsymbol{\tau}$-matrices as follows:

$$\begin{aligned} V = V_a(r) + V_\sigma(r)(\boldsymbol{\sigma}^1\boldsymbol{\sigma}^2) + V_\tau(r)(\boldsymbol{\tau}^1\boldsymbol{\tau}^2) + V_{\sigma\tau}(\boldsymbol{\sigma}^1\boldsymbol{\sigma}^2)(\boldsymbol{\tau}^1\boldsymbol{\tau}^2)& \\ +V_{Td}(r)S_{12} + V_{T\tau}(\boldsymbol{\tau}^1\boldsymbol{\tau}^2)S_{12}.& \end{aligned} \tag{23.7}$$

Its coefficients are related to the earlier ones by

$$\begin{array}{lcllcl} V_a &=& V_W+\frac{1}{2}V_B-\frac{1}{2}V_H-\frac{1}{4}V_M, & V_\sigma &=& \frac{1}{2}V_B-\frac{1}{4}V_M \\ V_\tau &=& -\frac{1}{2}V_H-\frac{1}{4}V_M, & V_{\sigma\tau} &=& -\frac{1}{4}V_M \\ V_{Td} &=& V_{T\omega}-\frac{1}{2}V_{TM}, & V_{T\tau} &=& -\frac{1}{2}V_{TM}. \end{array} \tag{23.8}$$

---

[1] Notation: ${}^J_SL$ where L is the orbital angular momentum, S the combined spin, and J the total angular momentum.

TABLE 23.2 Action of spin and isospin operators in the expansion (23.7).

	even l		odd l	
	triplet	singlet	triplet	singlet
$\boldsymbol{\sigma}^1\boldsymbol{\sigma}^2$	-3	1	-3	1
$\boldsymbol{\tau}^1\boldsymbol{\tau}^2$	1	-3	-3	1
$(\boldsymbol{\sigma}^1\boldsymbol{\sigma}^2)(\boldsymbol{\tau}^1\boldsymbol{\tau}^2)$	-3	-3	9	1

In 1937, Wigner[2] observed that if the spin-orbit forces were small and Wigner and Majorana forces dominant, the potential could be written as

$$V = V_1(r) + V_2(r)(1+\boldsymbol{\sigma}^1\boldsymbol{\sigma}^2)(1+\boldsymbol{\tau}^1\boldsymbol{\tau}^2) \tag{23.9}$$

and would be invariant under spin rotations, isospin rotations, and the extension of these two SU(2) groups to SU(4). Experimentally,

$$\frac{V_H}{V_M} \approx 0.4 - 0.5, \tag{23.10}$$

so there is relly quite large symmetry breaking. Still, the group has turned out to be quite useful in understanding nuclear spectra.

The group SU(4) is generated by the 15 4×4 matrices acting on a nucleon field $N_{\alpha\alpha'}$ with isospin index α $(\alpha = 1,2)$ and spin index α $(\alpha' = 1,2)$:

$$\frac{\boldsymbol{\tau}}{2}\times 1, \quad 1\times\frac{\boldsymbol{\sigma}}{2}, \quad \frac{\boldsymbol{\tau}}{2}\times\frac{\boldsymbol{\sigma}}{2}. \tag{23.11}$$

The commutation rules are given by the known ones for $\boldsymbol{\sigma}, \boldsymbol{\tau}$, an additional set of obvious commutation rules between the $\boldsymbol{\sigma}$'s and $\boldsymbol{\tau}$'s and the combined generators $(\boldsymbol{\tau}/2)\times(\boldsymbol{\sigma}/2)$ expressing their vector nature with respect to each subgroup, plus the new ones

$$\left[\frac{\tau^a\times\sigma^i}{2}, \frac{\tau^b\times\sigma^j}{2}\right] = i\delta_{ab}\epsilon_{ijk}1\times\frac{\sigma^k}{2} + i\epsilon_{abc}\delta_{ij}\frac{\tau^c}{2}\times 1. \tag{23.12}$$

If SU(4) is a good approximate symmetry of nuclear forces then nuclei should occur in irreducible multiplets of SU(4). Moreover, since both isospin and $\boldsymbol{\sigma}$ are invariant under space reflections, each multiplet should all have the same parity.

The fundamental representation of SU(4) is four-dimensional and denoted by 4. Its four components are identified with the four states of the nucleon as follows

$$N = \begin{pmatrix} p^{\uparrow} \\ p^{\downarrow} \\ n^{\uparrow} \\ n^{\downarrow} \end{pmatrix}, \tag{23.13}$$

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[2] E.P. Wigner and E. Feenberg, Phys. Rev. *51*, 106 (1937) and Rep. Progr. Phys. *8*, 274 (1941).

The higher representations are obtained as usual. One forms an appropriate multinucleon state of highest spin and isospin and applies the lowering operators

$$\frac{\tau^-}{2}\times 1,\quad 1\times\frac{\sigma^-}{2},\quad \frac{\tau^-\times\sigma^3}{4},\frac{\tau^3\times\sigma^-}{4},\frac{\tau^-\times\sigma^-}{4}. \tag{23.14}$$

to generate irreducible multiplets.
Consider the symmetric Young tableau $\square\square$ and take the state of highest weight in isospin and spin

$$|1,1;1,1\rangle \equiv |p^\uparrow p^\uparrow\rangle, \tag{23.15}$$

where the notation on the left-hand side specifies the isospins and spins T,S and their third components as $|T,T_3;S,S_3\rangle$.[3] From the state (23.15) we run through the entire isovector triplet of spin 1 by repeated application of the lowering operator τ^-. For these the other spin components are obtained by applying σ^-.
The application of $\tau^-/2$ to (23.15) gives the state

$$|1,0;1,1\rangle = \frac{1}{\sqrt{2}}|n^\uparrow p^\uparrow + p^\uparrow n^\uparrow\rangle \tag{23.16}$$

and $\sigma^-/2$ leads to

$$|1,0;1,0\rangle = \frac{1}{2}|n^\downarrow p^\uparrow + n^\uparrow p^\downarrow + p^\downarrow n^\uparrow + p^\uparrow n^\downarrow\rangle. \tag{23.17}$$

Since the two operators τ^-, σ^- are taken from the $\mathrm{SU}(2)_T\times\mathrm{SU}(2)_S$ subgroup, they do not change T,S. This is only possible by applying a proper SU(4) generator such as $\tau^-\times\sigma^-/4$. It creates the mixed state

$$\frac{1}{\sqrt{2}}|n^\downarrow p^\uparrow + p^\uparrow n^\downarrow\rangle. \tag{23.18}$$

Combining this with (23.17) we now form the state

$$|0,0;0,0\rangle = \frac{1}{\sqrt{4}}|n^\downarrow p^\uparrow - p^\downarrow n^\uparrow - n^\uparrow p^\downarrow + p^\uparrow n^\downarrow\rangle \tag{23.19}$$

which is orthogonal to (23.17) and has the property that

$$\begin{aligned}
\frac{\tau^-}{2}|0,0;0,0\rangle &= \frac{1}{2}|n^\downarrow n^\uparrow - n_\downarrow n^\uparrow - n^\uparrow n^\downarrow + n^\uparrow n^\downarrow\rangle = 0, & (23.20)\\
\frac{\sigma^-}{2}|0,0;0,0\rangle &= \frac{1}{2}|n^\downarrow n^\downarrow - p_\downarrow n^\downarrow - n^\downarrow p^\downarrow + p^\downarrow n^\downarrow\langle(= 0, & (23.21)
\end{aligned}$$

showing that it is a singlet under isospin and spin operations which was anticipated by the zeros in the ket on the left-hand side of (23.19). Thus we have found an irreducible decuplet of SU(4) with 10 states and the $[T,S]$ decomposition

$$10 = [1,1] + [0,0]. \tag{23.22}$$

---

[3] In accordance with the names for the isospin and spin matrices $\boldsymbol{\tau},\boldsymbol{\sigma}$ we denote here the iospin operators by T rather than I, as is customary in nuclear physics.

In addition, there is a six-dimensional representation 6 with the states

$$
\begin{aligned}
|0,0;1,1\rangle &= \frac{1}{\sqrt{2}}|p^{\uparrow}n^{\uparrow} - n^{\uparrow}p^{\uparrow}\rangle, \\
\frac{\sigma^-}{2}|0,0;1,1\rangle &= \frac{1}{\sqrt{2}}|p^{\downarrow}n^{\uparrow} + p^{\uparrow}n^{\downarrow} - n^{\downarrow}p^{\uparrow} - n^{\uparrow}p^{\downarrow}\rangle = \sqrt{2}|0,0;1,0\rangle, \\
\frac{\sigma^-}{2}|0,0;1,1\rangle &= (p^{\downarrow}n^{\downarrow} - n^{\downarrow}p^{\downarrow}) = \sqrt{2}|0,0;1,-1\rangle \\
\frac{\sigma^- \times \tau^-}{4}|0,0;1,1\rangle &= \frac{1}{\sqrt{2}}|n^{\downarrow}n^{\uparrow} - n^{\uparrow}n^{\downarrow}\rangle = |1,-1;0,0\rangle \\
\frac{\tau^+}{2}|1,-1;0,0\rangle &= \frac{1}{\sqrt{2}}|p^{\downarrow}n^{\uparrow} + n^{\downarrow}p^{\uparrow} - p^{\uparrow}n^{\downarrow} - n^{\uparrow}p^{\downarrow}\rangle = \sqrt{2}|1,0;0,0\rangle \\
\frac{\tau^+}{2}|1,0;0,0\rangle &= |p^{\downarrow}p^{\uparrow} - p^{\uparrow}p^{\downarrow}\rangle = \sqrt{2}|1,1;0,0\rangle.
\end{aligned}
\tag{23.23}
$$

These have the $[T,S]$ content

$$6 = [1,0] + [0,1]. \tag{23.24}$$

These are all irreducible contents in the tensor product, i.e.,

$$4 \times 4 = 10 + 6. \tag{23.25}$$

The deuteron is a state in the irreducible representation 6. It has $[T,S] = [0,1]$, i.e., it is an isosinglet vector particle transforming like the SU(4) generator $\boldsymbol{\tau}/2 \times 1$. If SU(4) is to be a good approximate symmetry, there should also be a partner $[1,0]$, i.e., a spin-zero isotriplet transforming like the SU(4) generator $1 \times \boldsymbol{\sigma}/2$. This does not really exist. However, the singlet NN scattering length is very large in the $T = 1$ state indicating a bound state just around the cut of the two-particle continuum in the energy plane. The symmetry breaking prevents these SU(4) partners to appear as physical particles.[4]

In elementary-particle physics, the group SU(4) combining isospin and spin has played quite an important historical role. There, up and down quarks with spin up and down are identified with the representation 4 of SU(4):

$$4 = \begin{pmatrix} u^{\uparrow} \\ u^{\downarrow} \\ d^{\uparrow} \\ d^{\downarrow} \end{pmatrix}. \tag{23.26}$$

For mesons, the representation 15 in $4 \times \bar{4} = 15 + 1$ extends the isospin triplet pseudoscalars π^+, π^0, π^-, which transform in the same way as the generators of the isospin subgroup τ^a, by the vector mesons ρ^+, ρ^0, ρ^-, which transform like $\tau^a \times \sigma^i$,

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[4] For more detail see the paper A. Franzini, A. Radicati, Phys. Lett **6**, 322 (1963).

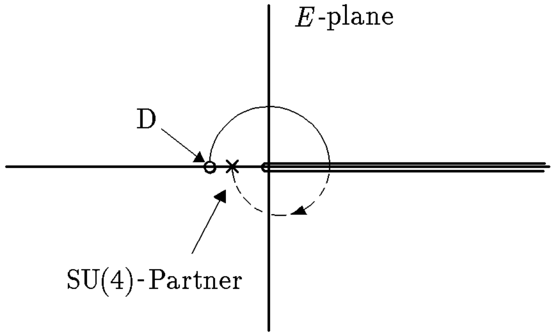


FIGURE 23.1 Pole position of the would-be SU(4) partner of the deuteron with spin-1 and isospin-0. It is close to the D-pole but not a particle since it hides in the complex energy plane just below the two-particle cut.

plus an isosinglet σ^i which is identified with the ω meson. The symmetry breaking, however, is extremely large since

$$\begin{aligned} m_\pi &\approx 135\text{ MeV}, \\ m_\rho &\approx 770\text{ MeV}, \\ m_\omega &\approx 783\text{ MeV}. \end{aligned} \tag{23.27}$$

For the nucleons p, n, the SU(4) symmetry is much better. Taking three up and down quarks with spin up and down, the three Young tableaux

$$\begin{array}{ccc}\square\square\square\end{array}, \qquad \begin{array}{l}\square\square\\ \square\end{array}, \qquad \begin{array}{c}\square\\ \square\\ \square\end{array}, \tag{23.28}$$

correspond, according to the general dimension formula,

$$\frac{n(n+1)(n+2)}{6}, \quad \frac{(n-1)n(n+1)}{3}, \quad \frac{n(n-1)(n-2)}{6} \tag{23.29}$$

to one symmetric 20, two mixed 20, and one antisymmetric 4 representation. Actually, the latter 4 is equivalent the complex conjugate $\bar{4}$ of the fundamental representation. To see this we note that the completely antisymmetric representation

$$\begin{array}{c}\square\\ \square\\ \square\\ \square\end{array}$$

of rank 4 is one-dimensional which means that the antisymmetric 4 must have met with a $\bar{4}$ to form an invariant.

In order to find the isospin and spin contents of the representations (23.28), we write the SU(4) index as α, α' where α are the two isospin indices and α' the spin indices. The representation 4 is a doublet with respect to each subgroup

$$\boxed{a\alpha} = 2 \times 2. \tag{23.30}$$

The Young tableau $\square\square = 10$ is symmetric under the simultaneous exchange of both indices. Hence, with respect to the two subgroups it can become a product of symmetric tensors or antisymmetric tensor

$$\begin{array}{ccccccccc} \boxed{a\alpha}\boxed{b\beta} & = & \boxed{a}\boxed{b} & \times & \boxed{\alpha}\boxed{\beta} & + & \begin{array}{c}\boxed{a}\\ \boxed{b}\end{array} & \times & \begin{array}{c}\boxed{\alpha}\\ \boxed{\beta}\end{array} \\ 10 & & 3 & & 3 & & 1 & & 1 \end{array} \tag{23.31}$$

Similarly

$$\begin{array}{ccccccccc} \begin{array}{c}\boxed{a\alpha}\\ \boxed{b\beta}\end{array} & = & \begin{array}{c}\boxed{a}\\ \boxed{b}\end{array} & \times & \boxed{\alpha}\boxed{\beta} & + & \boxed{a}\boxed{b} & \times & \begin{array}{c}\boxed{\alpha}\\ \boxed{\beta}\end{array} \\ 6 & = & 1 & & 3 & & 3 & & 1 \end{array} \tag{23.32}$$

To obtain all irreducible tensors of rank 3 we multiply $\square\square$ and $\begin{array}{c}\square\\ \square\end{array}$ by another box and find within SU(4) the decomposition

$$\begin{array}{ccccccc} \square\square & \times & \square & = & \square\square\square & + & \begin{array}{l}\square\square\\ \square\end{array} \\ 10 & & 4 & & 20 & & 20 \end{array} \ . \tag{23.33}$$

and

$$\begin{array}{ccccccc} \begin{array}{c}\square\\ \square\end{array} & \times & \square & = & \begin{array}{l}\square\square\\ \square\end{array} & + & \begin{array}{c}\square\\ \square\\ \square\end{array} \\ 6 & & 4 & & 20 & & \bar{4} \ . \end{array} \tag{23.34}$$

As far as the isospin and spin contents are concerned, we multiply the decomposition (23.31) of the 10 by

$$\begin{array}{ccccc} \square & = & \square & \times & \square \\ 4 & & 2 & & 2 \end{array} \ . \tag{23.35}$$

Thus the product 10×4 contains the isospin spin products

$$\begin{array}{ccccccc} \square\square & \times & \square & = & \square\square\square & + & \begin{array}{l}\square\square\\ \square\end{array} \\ 3 & & 2 & & 4 & & 2 \end{array} \tag{23.36}$$

$$\begin{array}{ccccc} \begin{array}{c}\square\\ \square\end{array} & \times & \square & = & \begin{array}{l}\square\square\\ \square\end{array} \\ 1 & & 2 & & 2 \end{array} \tag{23.37}$$

In the second case there is only one product since $\begin{array}{c}\square\\ \square\end{array}$ is one-dimensional. Hence we can decompose 10×4 as follows

$$\begin{array}{ccccccccccccccc} \square\square & \times & \square & = & (& \square\square\square & + & \begin{array}{l}\square\square\\ \square\end{array} &) & \times & (& \square\square\square & + & \begin{array}{l}\square\square\\ \square\end{array} &) \\ 10 & & 4 & & & 4 & & 2 & & & & 4 & & 2 & \end{array} \tag{23.38}$$

$$+\ \underset{2}{\yng(2,1)} \times \underset{2}{\yng(2,1)} \tag{23.39}$$

On the left-hand side, the product reduces to

$$\underset{20}{\yng(3)} + \underset{20}{\yng(2,1)} \tag{23.40}$$

It is easy to read off which products on the right-hand side belong to these two representations.

$$\underset{20}{\yng(3)} = \underset{4}{\yng(3)} \times \underset{4}{\yng(3)} + \underset{2}{\yng(2,1)} \times \underset{2}{\yng(2,1)} \tag{23.41}$$

$$\begin{aligned} \underset{20}{\yng(2,1)} &= \underset{4}{\yng(3)} \times \underset{2}{\yng(2,1)} + \underset{2}{\yng(2,1)} \times \underset{4}{\yng(3)} \\ &+ \underset{2}{\yng(2,1)} \times \underset{2}{\yng(2,1)} \end{aligned} \tag{23.42}$$

Thus the symmetric 20 consists of a spin-$\frac{1}{2}$ isospin-$\frac{1}{2}$ and a spin-$\frac{3}{2}$ isospin-$\frac{3}{2}$ multiplet. They are associated with the following particles. The spin-$\frac{1}{2}$ isospin-$\frac{1}{2}$ states are the two isospin states of the nucleon p, n. The spin $\frac{3}{2}$ isospin $\frac{3}{2}$ states contain the first pion nucleon reson $\Delta(1230)$ plus its isospin partners with the charge states $-, 0, +, ++$. All particles have intrinsic parity $+$.

The mixed 20 consists of a spin-$\frac{3}{2}$ isospin-$\frac{1}{2}$, a spin-$\frac{1}{2}$ isospin-$\frac{3}{2}$, and spin-$\frac{1}{2}$ isospin-$\frac{1}{2}$ multiplet. Also these states are found experimentally in pion-nucleon scattering as resonances of negative parity. The isotriplet spin-$\frac{1}{2}$ states are the P wave resonances of spin-parity $S^P = \frac{1}{2}^-$ called $\Delta(1620)$, the isodoublet spin-$\frac{3}{2}$ states are the P wave $\frac{3}{2}^- N(1520)$ resonances, and the isodoublet spin $\frac{1}{2}$ states are the P wave $\frac{1}{2}^-$ $N(1650)$ resonances.

The content of the antisymmetric SU(4) representation

$$\yng(1,1,1) = \bar{4}$$

is obviously 2×2 , i.e. an isospin $\frac{1}{2}$ spin $\frac{1}{2}$ multiplet. It is associated with the $N(1440)$ pion nucleon resonance of spin-parity $\frac{1}{2}^+$.

23.2 SU(6) Symmetry of Strong Interactions

With the success of the approximate symmetry SU(4) in nuclear and particle the question arose whether there exists an extension of the symmetry group which includes also the internal symmetry SU(3). The three quarks with spin up and down form a sextet of particles

$$q = \begin{pmatrix} u^{\uparrow} \\ u^{\downarrow} \\ d^{\uparrow} \\ d^{\downarrow} \\ s^{\uparrow} \\ s^{\downarrow} \end{pmatrix} . \tag{23.43}$$

Hence the most straightforward extension would be SU(6). This group is generated by the 35 matrices

$$\frac{\lambda^a}{2} \times 1, \quad 1 \times \frac{\sigma^i}{2}, \quad \frac{\lambda^a}{2} \times \frac{\sigma^i}{2}. \tag{23.44}$$

The only non-trivial commutation rules are

$$\begin{aligned} \left[\frac{\lambda^a \times \sigma^i}{2}, \frac{\lambda^b \times \sigma^j}{2} \right] &= i d_{abc} \epsilon_{ijk} \frac{1}{2} \lambda^c \times \sigma^k + i f_{abc} \delta_{ij} \frac{1}{2} \lambda^c \times 1 \\ &\quad + i \frac{2}{3} \delta_{ab} \epsilon_{ijk} 1 \times \frac{1}{2} \sigma^k . \end{aligned} \tag{23.45}$$

Since in SU(4), the representation 4 × 4 contained the pseudoscalar π and vector mesons ρ, ω, we expect the representation $6 \times \bar{6}$ to extend these multiplets by the missing SU(3) partners. The representation $6 \times \bar{6}$ decomposes into $35 + 1$ with the particles in the 35 representation having the transformation properties of the 35 group generators (23.44). Thus there is now an SU(3) octet of pseudoscalar mesons which transform like the generators $\lambda^a \times 1/2$. There is a further SU(3) octet of vector mesons ρ, ω, K^*. They form 24 states which transforms like the generators $\lambda^a \times \sigma^i/2$, and there is an SU(3) singlet vector meson $\varphi(1020)$ which transforms like the three generators $1 \times \sigma^i/2$. These meson multiplets are quite widely separated in mass and the symmetry SU(6) is strongly broken. Still, the approximate symmetry group organizes nicely all the most important low-lying meson states as illustrated in Fig. 23.2.

As in the case of SU(4) symmetry, the situation is much better for the baryons. The nucleons and their strange partners as well as the first nucleon resonances and their strange partners lie all in one irreducible multiplets of three-quark states. They decompose as follows:

$$\underset{6}{\square} \times \underset{6}{\square} \times \underset{6}{\square} = \underset{56}{\square\square\square} + 2 \times \underset{70}{\begin{array}{l}\square\square \\ \square\end{array}} + \underset{20}{\begin{array}{c}\square \\ \square \\ \square\end{array}} \tag{23.46}$$

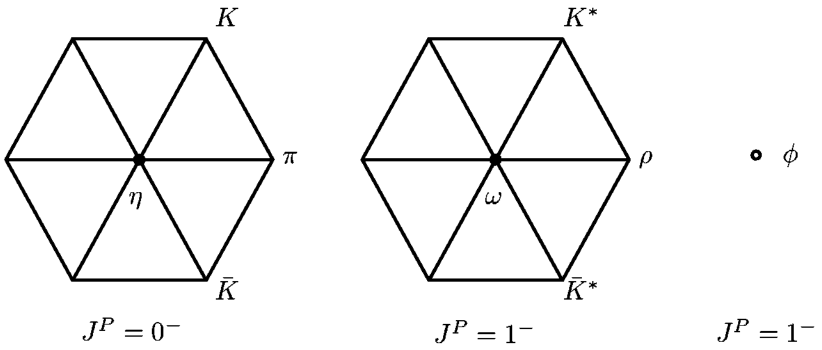


FIGURE 23.2 The pseudoscalar and vector mesons of the 35 representation of SU(6).

In order to find the SU(3) and spin contents of these multiplets we decompose, as in the case of SU(4),

$$\underset{6}{\boxed{\mathrm{a}\alpha}} = \underset{3}{\boxed{\mathrm{a}}} \times \underset{2}{\boxed{\alpha}} \tag{23.47}$$

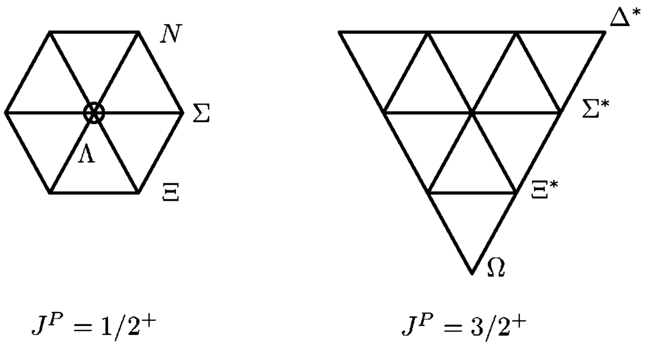
and form the symmetric and antisymmetric products of two representations 6. They are 21- and 15-dimensional and their SU(3) and spin contents are given by

$$\underset{21}{\boxed{\mathrm{a}\alpha}\boxed{\mathrm{b}\beta}} = \underset{6}{\boxed{\mathrm{a}}\boxed{\mathrm{b}}} \times \underset{3}{\boxed{\alpha}\boxed{\beta}} + \underset{\bar 3}{\begin{array}{c}\boxed{\mathrm{a}}\\ \boxed{\mathrm{b}}\end{array}} \times \underset{1}{\begin{array}{c}\boxed{\alpha}\\ \boxed{\beta}\end{array}}$$

$$\underset{15}{\begin{array}{c}\boxed{\mathrm{a}\alpha}\\ \boxed{\mathrm{b}\beta}\end{array}} = \underset{6}{\boxed{\mathrm{a}}\boxed{\mathrm{b}}} \times \underset{1}{\begin{array}{c}\boxed{\alpha}\\ \boxed{\beta}\end{array}} + \underset{\bar 3}{\begin{array}{c}\boxed{\mathrm{a}}\\ \boxed{\mathrm{b}}\end{array}} \times \underset{3}{\boxed{\alpha}\boxed{\beta}}$$

Multiplying the 21 by a further 6 we find

$$\begin{aligned}
\underset{21}{\boxed{}\boxed{}} \times \underset{6}{\boxed{}} &= \underset{56}{\boxed{}\boxed{}\boxed{}} + \underset{70}{\begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}}\\
&= \left(\underset{10}{\boxed{}\boxed{}\boxed{}} + \underset{8}{\begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}}\right) \times \left(\underset{4}{\boxed{}\boxed{}\boxed{}} + \underset{2}{\begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}}\right)\\
&\quad + \left(\underset{1}{\begin{array}{c}\boxed{}\\ \boxed{}\\ \boxed{}\end{array}} \times \underset{8}{\begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}}\right) \times \underset{2}{\begin{array}{l}\boxed{}\boxed{}\\ \boxed{}\end{array}}
\end{aligned} \tag{23.48}$$



$J^P = 1/2^+$ $J^P = 3/2^+$

FIGURE 23.3 The SU(3) content of the particles in the 56 representation of SU(6) containing the $J^P = 1/2^+$ nucleons and the $J^P = 3/2^+$ resonances.

It is then easy to read off the SU(3) and spin contents on the right-hand side

$$
\begin{aligned}
\underset{56}{\ydiagram{3}} &= \underset{10}{\ydiagram{3}} \times \underset{4}{\ydiagram{3}} + \underset{8}{\ydiagram{2,1}} \times \underset{2}{\ydiagram{2,1}} \\
\underset{70}{\ydiagram{2,1}} &= \underset{10}{\ydiagram{3}} \times \underset{2}{\ydiagram{2,1}} + \underset{8}{\ydiagram{2,1}} \times \underset{4}{\ydiagram{3}} \\
&\quad + \underset{8}{\ydiagram{2,1}} \times \underset{2}{\ydiagram{2,1}} + \underset{1}{\ydiagram{1,1,1}} \times \underset{2}{\ydiagram{2,1}}
\end{aligned}
\tag{23.49}
$$

Thus the 56 consists of a decuplet of spin $\frac{3}{2}$ and an octet of spin $\frac{1}{2}$ states. These can be associated with the decuplet of nucleon resonances and the nucleon octet, all of positive parity as shown in Fig. 23.3.

The 70 consists of a decuplet of spin $\frac{1}{2}$, an octet of spin $\frac{3}{2}$, an octet of spin $\frac{1}{2}$, thus extending the isospin multiplets of negative parity, assigned in the SU(4) case, to the SU(3) multiplets shown in Fig. 23.4.

FIGURE 23.4 The nucleon resonance of negative parity in the 70 representation of SU(6).

The SU(3) × SU(2) contents of the antisymmetric SU(6) representation

$$\underset{20}{\ydiagram{1,1,1}}$$

are easily written down as

$$\underset{20}{\begin{array}{c}\square\\\square\\\square\end{array}} = \underset{8}{\square\square\square} \times \underset{2}{\begin{array}{c}\square\\\square\\\square\end{array}} + \underset{1}{\begin{array}{c}\square\\\square\\\square\end{array}} \times \underset{4}{\square\square\square} \tag{23.50}$$

The octet states may be the spin $\frac{1}{2}$ particles of positive parity shown in Fig. 23.5. The SU(3) singlet $\frac{3}{2}^+$ partner of them has not yet been found.

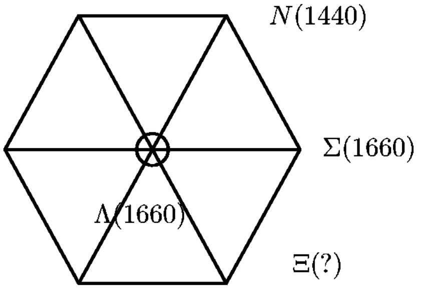


FIGURE 23.5 Octet of spin-parity $\frac{1}{2}^+$ baryons.

Let us now study the states of the 56 representation in more detail. The state of highest weight is the $\Delta^{++}(1235)$ resonance of spin $\frac{3}{2}$

$$\Delta^{++}(1235)^{\uparrow\uparrow} = |u^\uparrow u^\uparrow u^\uparrow\rangle. \tag{23.51}$$

By lowering spin and isospin once one obtains

$$\begin{aligned}\Delta^{+}(1235)^{\uparrow} = \; & \frac{1}{3}|d^\downarrow u^\uparrow u^\uparrow + u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow \\ & + d^\uparrow u^\downarrow u^\uparrow + u^\uparrow d^\downarrow u^\uparrow + u^\uparrow u^\downarrow d^\uparrow \\ & + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow + u^\uparrow u^\uparrow d^\downarrow\rangle.\end{aligned} \tag{23.52}$$

By applying the operator $\lambda^3\sigma^3$ to this we find

$$\begin{aligned}&\lambda^3\sigma^3\Delta^{+}(1235)^{\uparrow} = \frac{1}{3}|3(d^\downarrow u^\uparrow u^\uparrow + u^\uparrow d^\downarrow u^\uparrow + u^\uparrow u^\uparrow d^\downarrow) \\ &-(u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow + u^\uparrow u^\downarrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow))\rangle.\end{aligned} \tag{23.53}$$

This must be a mixture of $\Delta^{+}(1235)^{\uparrow}$ and a proton $p^\uparrow$.

Since the proton is orthogonal to $\Delta^{+}(1235)^{\uparrow}$ we can immediately identify the normalized proton state as

$$\begin{aligned}p^\uparrow = \; & \frac{\sqrt{2}}{3}|d^\downarrow u^\uparrow u^\uparrow + u^\uparrow d^\downarrow u^\uparrow + u^\uparrow u^\uparrow d^\downarrow \\ & -\frac{1}{2}(u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow u^\downarrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow))\rangle.\end{aligned} \tag{23.54}$$

Applying the isospin lowering operator we obtain the neutron:

$$\begin{aligned} n^\uparrow = & -\frac{\sqrt{2}}{3}|d^\uparrow d^\uparrow u^\downarrow + d^\uparrow u^\downarrow d^\uparrow + u^\downarrow d^\uparrow d^\uparrow \\ & -\frac{1}{2}(d^\downarrow u^\uparrow d^\uparrow + d^\downarrow d^\uparrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow d^\downarrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow u^\uparrow d^\downarrow))\rangle . \end{aligned} \tag{23.55}$$

As an interesting consequence of SU(6) one may calculate the ratio between the magnetic moment of neutron and proton. For this one assumes that the magnetic moment operator transforms under SU(3) like the charge operator which is given by the generators

$$Q = \lambda^Q = \frac{1}{2}\left(\lambda^3 + \frac{1}{\sqrt{3}}\lambda^8\right) . \tag{23.56}$$

Under rotations, it must transform like a spin operator $\propto \boldsymbol{\sigma}$. Thus the magnetic moment operator should be proportional to the following generator in SU(6)

$$\boldsymbol{\mu} = \frac{1}{2}(\lambda^3 + \frac{1}{\sqrt{3}}\lambda^8) \times \boldsymbol{\sigma}. \tag{23.57}$$

One now applies the third component of this,

$$\mu_3 \equiv \mu = \frac{1}{2}(\lambda^3 + \frac{1}{\sqrt{3}}\lambda^8) \times \sigma^3, \tag{23.58}$$

to the quark states and finds the eigenvalues shown in Table 23.3. Specifically, the application gives

TABLE 23.3 Eigenvalues of charge and other operators on quark states.

q	$u^\uparrow$	$u^\downarrow$	$d^\uparrow$	$d^\downarrow$	$s^\uparrow$	$s^\downarrow$
$\lambda^3 \times \sigma^3$	1	-1	1	-1	0	0
$\lambda^8 \times \sigma^3/\sqrt{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{2}{3}$	$\frac{2}{3}$
$Q \times \sigma_3$	$\frac{2}{3}$	$-\frac{2}{3}$	$-\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	$\frac{1}{3}$

$$\begin{aligned} \mu p^\uparrow = & \frac{\sqrt{2}}{3}\bigg|\frac{5}{3}(d^\downarrow u^\uparrow u^\uparrow + u^\uparrow d^\downarrow u^\uparrow + u^\uparrow u^\uparrow d^\downarrow) \\ & -\frac{1}{2}\left(-\frac{1}{3}\right)(u^\downarrow d^\uparrow u^\uparrow + u^\downarrow u^\uparrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow u^\downarrow d^\uparrow + d^\uparrow u^\uparrow u^\downarrow + u^\uparrow d^\uparrow u^\downarrow)\bigg\rangle, \end{aligned} \tag{23.59}$$

$$\begin{aligned} \mu_3 n^\uparrow = & \frac{\sqrt{2}}{3}\bigg| -\frac{4}{3}(d^\uparrow d^\uparrow u^\downarrow + d^\uparrow u^\downarrow d^\uparrow + u^\downarrow d^\uparrow d^\uparrow) \\ & -\frac{1}{2}\left(\frac{2}{3}\right)(d^\downarrow u^\uparrow d^\uparrow + d^\downarrow d^\uparrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow d^\downarrow u^\uparrow + u^\uparrow d^\uparrow d^\downarrow + d^\uparrow u^\uparrow d^\downarrow)\bigg\rangle, \end{aligned} \tag{23.60}$$

so that we find the matrix elements

$$\begin{aligned} \langle p^\uparrow|\mu|p^\uparrow\rangle &= \frac{2}{9}\left(\frac{5}{3}\cdot 3 - \frac{1}{3}\cdot\frac{6}{4}\right) = 1, \\ \langle n^\uparrow|\mu|n^\uparrow\rangle &= \frac{2}{9}\left(-\frac{4}{3}\cdot 3 + \frac{2}{3}\cdot\frac{6}{4}\right) = -\frac{2}{3}. \end{aligned} \tag{23.61}$$

This yields the ratio of magnetic moments

$$\frac{\mu_n}{\mu_p} = -\frac{2}{3}. \tag{23.62}$$

Experimentally, the magnetic moments are

$$\begin{aligned} \mu_p &= 2.7928444 \pm 0.0000011, \\ \mu_n &= -1.91304308 \pm 0.00000054, \end{aligned} \tag{23.63}$$

in units of $c\hbar/2m_pc = 505 \times 10^{-24}$ erg/Gauss. Thus the ratio is $\approx -2.055/3$, in excellent agreement with the SU(6) prediction (23.62).

By the same method one can calculate all rates of the radiative decays of the decuplet resonances $10 \longrightarrow 8+\gamma$ in terms of only one unknown overall size parameter.

The possibility of predicting the ratio of the magnetic moments is due to the fact that in the irreducible multiplet 56 of the symmetry group SU(6), the SU(3) octet operator $\lambda^a \times \sigma^3/2$ has, between the octet states of nucleons, a specific ratio of symmetric and antisymmetric couplings (which within SU(3) would be arbitrary). Let us express the two couplings in terms of the irreducible matrix elements F and D as follows

$$\begin{aligned} \langle b|\frac{\lambda^a}{2} \times \sigma^3|c\rangle &= F\cdot(-if_{ab^*c}) + D\cdot(d_{ab^*c}) \\ &\equiv F\cdot(F_a)_{b^*c} + D\cdot(D_a)_{b^*c}. \end{aligned} \tag{23.64}$$

Then we find between protons with the octet components $(4+i\sqrt{5})/\sqrt{2}$

$$(F_3)_{pp} = f_{345} = \frac{1}{2}, \quad (D_3)_{pp} = d_{344} = \frac{1}{2}, \tag{23.65}$$

and between neutrons with the components $(6+i7)/\sqrt{2}$

$$(F_3)_{nn} = -f_{367} = -\frac{1}{2}, \quad (D_3)_{nn} = d_{366} = -\frac{1}{2}. \tag{23.66}$$

The eighths components of F_a, D_a have the matrix elements

$$\begin{array}{ll} (F_8)_{pp} = f_{845} = \sqrt{\frac{3}{2}}, & (D_8)_{pp} = d_{866} = -\frac{1}{2\sqrt{3}} \\ (F_8)_{nn} = f_{867} = \sqrt{\frac{3}{2}}, & (D_8)_{nn} = d_{866} = -\frac{1}{2\sqrt{3}}. \end{array} \tag{23.67}$$

The matrix elements of the magnetic moment operator

$$\mu_3 \equiv \mu = \lambda^Q \times \sigma^3 \equiv \frac{1}{2}(\lambda^3 + \frac{1}{\sqrt{3}}\lambda^8)\sigma^3 \tag{23.68}$$

are therefore given in terms of the irreducible matrix elements F and D by

$$\begin{aligned} \langle p|\mu|p\rangle &= F\cdot\left(\frac{1}{2}+\frac{1}{2}\right) + D\cdot\left(\frac{1}{2}-\frac{1}{6}\right) = \left(F+\frac{1}{3}D\right), \\ \langle n|\mu_3|n\rangle &= F\cdot\left(-\frac{1}{2}+\frac{1}{2}\right) + D\cdot\left(-\frac{1}{2}-\frac{1}{6}\right) = -\frac{2}{3}D. \end{aligned} \tag{23.69}$$

The ratio is

$$\frac{\langle p|\mu|p\rangle}{\langle n|\mu|n\rangle} = \frac{F/D + \frac{1}{3}}{-\frac{2}{3}}. \qquad (23.70)$$

This holds on the basis of only SU(3) symmetry. Inserting the SU(6) result (23.62) we see that SU(6) fixes the F/D ratio

$$F/D = \frac{2}{3}. \qquad (23.71)$$

The absolute values of the irreducible matrix elements of the operators

$$\frac{\lambda^3}{2} \times \sigma^3, \quad \frac{\lambda^8}{2} \times \sigma^3, \qquad (23.72)$$

are also known from the above calculation [Eq. (23.61)]:

$$F + D\frac{1}{3} = 1, \quad -\frac{2}{3}D = -\frac{2}{3} \qquad (23.73)$$

so that

$$F = \frac{2}{3}, \quad D = 1. \qquad (23.74)$$

It is straight-forward to calculate the magnetic moment of any other members of the octet, for instance of $\Sigma^+ \hat{=} (1 + i2)/\sqrt{2}$:

$$\begin{aligned}
\langle \Sigma^+|\mu|\Sigma^+\rangle &= F \cdot \left(-if_{Q12}\right) + D \cdot d_{Q11} \\
&= F \cdot \left[\frac{1}{2}\left(f_{312} + \frac{1}{\sqrt{3}} f_{812}\right)\right] + D \cdot \left[-\frac{1}{2}\left(d_{311} + \frac{1}{\sqrt{3}} d_{811}\right)\right] \\
&= \frac{1}{2}F + \frac{1}{6}D = \frac{1}{2}. \qquad (23.75)
\end{aligned}$$

This implies the ratio

$$\frac{\langle p|\mu|p\rangle}{\langle \Sigma^+|\mu|\Sigma^+\rangle} = 2. \qquad (23.76)$$

In fact, the fastest way to find the F/D ratio is by calculating from the SU(6) wave functions the matrix elements of $\lambda^3 \times \sigma^3/2$. Between protons we find immediately

$$\langle p|\frac{\lambda^3}{2} \times \sigma^3|p\rangle = \frac{5}{6}. \qquad (23.77)$$

Using the wave function

$$\begin{aligned}
|\Sigma^{+\uparrow}\rangle = \frac{\sqrt{2}}{3}| &\left(u^\uparrow u^\uparrow s^\downarrow + u^\uparrow s^\downarrow u^\uparrow + s^\downarrow u^\uparrow u^\uparrow\right) \qquad (23.78) \\
&-\frac{1}{2}(u^\uparrow u^\downarrow s^\uparrow + u^\downarrow s^\uparrow u^\uparrow + s^\uparrow u^\uparrow u^\downarrow + u^\downarrow u^\uparrow s^\uparrow + u^\uparrow s^\uparrow u^\downarrow + s^\uparrow u^\downarrow u^\uparrow))\rangle.
\end{aligned}$$

we obtain

$$\langle\Sigma^+|\frac{\lambda^3}{2}\times\sigma^3|\Sigma^+\rangle=\frac{2}{3}. \tag{23.79}$$

In terms of the irreducible matrix elements F, D, the corresponding matrix elements would be in general

$$\begin{aligned}\langle p|\frac{\lambda^3}{2}\times\sigma^3|p\rangle &= \frac{F}{2}+\frac{D}{2},\\ \langle\Sigma^+|\frac{\lambda^3}{2}\times\sigma^3|p\rangle &= F.\end{aligned} \tag{23.80}$$

Hence we identify, once more,

$$F=\frac{2}{3},\quad D=1. \tag{23.81}$$

The magnetic moment μ for the transition $p\rightarrow\Delta$ is found by multiplying $\mu|p^\uparrow\rangle$ from the left by $\langle\Delta^{+\uparrow}|$. This gives

$$\mu^*\equiv\langle\Delta^{+\uparrow}|\mu|p^\uparrow\rangle=\frac{\sqrt{2}}{9}\left[\frac{5}{3}\cdot 3+\frac{1}{6}\cdot 6\right]=\frac{2}{3}\sqrt{2}. \tag{23.82}$$

We therefore have the SU(6) prediction

$$\mu^*=\frac{2}{3}\sqrt{2}\mu_p. \tag{23.83}$$

Experimentally one finds from the $\Delta(1236)$ resonance in the photoproduction cross section

$$\gamma+p\rightarrow\pi^0+p \tag{23.84}$$

the value

$$\mu^*_{exp}\approx(1.28-0.01)\cdot\mu^*. \tag{23.85}$$

This is not in quite as good agrement as the proton-to-neutron ratio. We must, however, keep in mind that the symmetry SU(6) is significantly broken and that the comparison with the data requires taking matrix elements of μ between states whose normalization factors can depend on the masses of the particles. Thus one is bound to commit errors of the order of the relative mass differences within the experimental multiplets, here between the $\Delta(1232)$ and the proton $p(938)$. These can easily accounts for the 28 % discrepancy in the magnetic moment prediction (23.85).

23.3 SU(6) and Current Algebra

Historically, the SU(6) symmetry had an important impact upon the development of the quark model. Since the symmetry is only approximate there was need to find a way of controlling the symmetry breaking corections. For the group SU(6) this has remained impossible, not so, however, for an important subgroup of SU(6) generated by $\lambda^a/2, \lambda^a\sigma^3/2$. It is called $\mathrm{SU}(3)_R \times \mathrm{SU}(3)_L$ and its generators are conveniently taken in the combinations

$$Q^a_\pm = \frac{\lambda^a}{2} \times \frac{(1 \pm \sigma^3)}{2}. \tag{23.86}$$

These generators are intimately related to the SU(3) × SU(3) current algebra which was discussed before in the context of chiral symmetries. The charges and axial charges observed in electromagnetic and weak interactions are related to $Q^a_\pm$ as follows:

$$Q^a = Q^a_+ + Q^a_-, \quad Q^a_5 = Q^a_+ - Q^a_-. \tag{23.87}$$

This relation makes it possible to calculate the symmetry breaking corrections in terms of experimentally observable quantities. The good SU(6) results for the magnetic moments were based on the prediction of the F/D ratio 2/3 and the ratio $\langle p|\mu|p\rangle / \langle \Delta^+|\mu|p\rangle = 2\sqrt{2}/3$. It is gratifying to observe that these predictions are already contained in the $\mathrm{SU}(3) \times \mathrm{SU}(3)_R$ subgroup of SU(6). The relation with the current algebra makes it then possible to calculate symmetry breaking corrections to these ratios.

The representations 56 and 70 of SU(6) have the following irreducible contents with respect to this subgroup

$$56 = \begin{pmatrix} \frac{3}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{3}{2} \\ (10,1) & (6,3)_{10} & -(3,6)_{10} & (1,10) \\ & (6,3)_8 & (3,6)_8 & \end{pmatrix} \tag{23.88}$$

$$70 = \begin{pmatrix} \frac{3}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{3}{2} \\ (8,1) & \frac{1}{\sqrt{2}}[(6,3) - (\bar{3}3)]_8 & \frac{1}{\sqrt{2}}[(3,6) + (3,5)]_8 & -(1,8) \\ & -(\bar{3},3)_8 & -(3,\bar{3})_8 & \\ & (\bar{3},3)_1 & -(3,\bar{6})_1 & \end{pmatrix}. \tag{23.89}$$

The columns in these matrices ordered according to the third component of the spin s_3 along the direction of the momentum of the particle which is indicated in the upper row and the subscripts denote the coupling of the two parts of $\mathrm{SU}(3)_R \times \mathrm{SU}(3)_L$ with respect to the ordinary SU(3) symmetry group generated by $Q^a_+ + Q^a_-$. Within this subgroup, the F/D ratio 2/3 is the F/D ratio found for the operator $Q^a_+ - Q^a_-$ between two $(6,3)_8$ representations and the transition $\Delta \longrightarrow p$ comes from the matrix element of $Q^a_+ - Q^a_- = \lambda^a\sigma^3/2$. The representation (6, 3) contains an SU(3) octet and a decuplet which can be identified with the nucleon octet and the first resonance decuplet at helicity $s_3 = 1/2$. between the octet and the decuplet parts of the irreducible representation (6, 3).

At this point it is useful to realize that the commutation rules of $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$ can be rephrased as sum rules for the irreducible matrix elements of Q^a, Q^a_5. Take, for example, the commutation rules between the axial charges

$$[Q^a_5, Q^b_5] = i f_{abc} Q^c. \tag{23.90}$$

Taking the commutators for $a = 1 + i2,\ b = a^*$

$$[Q_5^+, Q_5^-] = Q^3, \tag{23.91}$$

and sandwiching it between proton states, it gives

$$\langle p|Q_5^+ Q_5^-|p\rangle - \langle p|Q_5^- Q_5^+|p\rangle = \langle p|Q^3|p\rangle. \tag{23.92}$$

Inserting between the axial charges a complete set of intermediate states, we obtain

$$|\langle n|Q_5^-|p\rangle|^2 + |\langle \Delta^0|Q_5^-|p\rangle|^2 - |\langle \Delta^{++}|Q_5^+|p\rangle|^2 = \langle p|Q^3|p\rangle. \tag{23.93}$$

We now introduce irreducible matrix elements of the axial charge Q_5^a with respect to the SU(2) subgroup by defining between protons

$$\langle p|Q_5^3|p\rangle \equiv \frac{1}{2}G_A. \tag{23.94}$$

Then

$$\langle n|Q^-|p\rangle \equiv G_A \tag{23.95}$$

This can either be derived directly by using the generator $\lambda^- \sigma^3/2$ or via the Wigner-Eckart theorem for SU(2) vector operators. We only have to keep in mind that Q_5^3 creates the quantum numbers of π^0 while $Q_5^\pm$ creates those of $\sqrt{2}\pi^+, -\sqrt{2}\pi^-$ if we take π^+, π^0, π^- to satisfy the Condon-Shortley phase convention[5] We define further between a proton and a Δ-resonance

$$\langle \Delta^+|Q_T^3|p\rangle \equiv \frac{1}{\sqrt{2}}G^* \tag{23.96}$$

and have, by the Wigner-Eckart theorem,

$$\begin{aligned} \langle \Delta^{++}|Q_5^+|p\rangle &\equiv -\sqrt{\frac{3}{2}}G^*, \\ \langle \Delta^0|Q_5^-|p\rangle &= \frac{1}{\sqrt{2}}G^*. \end{aligned} \tag{23.97}$$

With the right-hand side of (23.93) being the isospin value of the proton 1/2 we obtain the sum rule

$$G_A^2 - G^{*2} = 1. \tag{23.98}$$

Similarly, we can take the commutator (23.91) between two Δ^{++} states and have the sum rule

$$|\langle p|Q_5^-|\Delta^{++}\rangle|^2 + |\langle \Delta^+|Q_5^-|\Delta^{++}\rangle| = 3. \tag{23.99}$$

Introducing the irreducible matrix element G_A^* of the axial charge between two Δ-states via

$$\langle \Delta^+|Q_5^0|\Delta^+\rangle = \frac{1}{2}G_A^* \tag{23.100}$$

---

[5] Verify this by applying $Q^\pm$ to Q^3 giving $\pm Q^\mp$.

so that, by the Wigner Eckart theorem,

$$\langle \Delta^+ | Q_5^- | \Delta^{++} \rangle = -\sqrt{3} G_A^*, \tag{23.101}$$

and (23.99) becomes

$$\frac{1}{2} G^{*2} + G_A^{*\,2} = 1. \tag{23.102}$$

Between p and Δ^+, finally, the commutator (23.91) becomes

$$\begin{aligned} &\langle \Delta^+ | Q_5^+ | n \rangle \langle n | Q_5^- | p \rangle + \langle \Delta^+ | Q_5^+ | \Delta^0 \rangle \langle \Delta^0 | Q_5^- | p \rangle \\ &\qquad - \langle \Delta^+ | Q_5^- | \Delta^{++} \rangle \langle \Delta^{++} | Q_5^+ | p \rangle = 0, \end{aligned} \tag{23.103}$$

which amounts to the sum rule

$$G^* G_A - 5 G_A^* G^* = 0. \tag{23.104}$$

The unique solution to these SU(2) × SU(2) sum rules is

$$G_A = \frac{5}{3}, \quad G^* = \frac{4}{3}, \quad G_A^* = \frac{1}{3}. \tag{23.105}$$

A more covariant looking derivation of these sum rules is possible by rewriting the matrix elements of Q_5^a for $a = 1, 2, 3$ between isospin $\frac{1}{2}$ and $\frac{3}{2}$ spinors as follows

$$\begin{aligned} NN: \quad (Q_5^a)_{mm'}^{11} &= G_A \chi^\dagger(m) \frac{\tau^a}{2} \chi(m') = G \frac{\sqrt{3}}{2} \langle \tfrac{1}{2}, m | 1, a; \tfrac{1}{2}, m' \rangle \\ \Delta N: \quad (Q_5^a)_{mm'}^{31} &= G^* \frac{\sqrt{3}}{2} \chi_a^\dagger(m) \chi(m') = G^* \frac{\sqrt{3}}{2} \langle \tfrac{3}{2}, m | 1, a; \tfrac{1}{2}, m' \rangle, \\ \Delta\Delta: \quad (Q_5^a)_{mm'}^{33} &= G_A^* \frac{3}{2} i \epsilon_{abc} \chi_b^+(m) \chi_c(m') = G_A^* \frac{\sqrt{15}}{2} \langle \tfrac{3}{2}, m | 1, a; \tfrac{3}{2}, m' \rangle. \end{aligned} \tag{23.106}$$

Here $\langle SM | s_1 m_1 s_2 m_2 \rangle$ are the usual SU(2) Clebsch-Gordan coefficients and χ_a are *Rarita-Schwinger isospinors*. They are obtained by coupling an ordinary isospinor χ with an isovector v_a by a Clebsch-Gordan coefficient

$$\chi_a(m) = \langle \tfrac{3}{2}, m | 1, m_1; \tfrac{1}{2}, m_2 \rangle v_a(m_1) \chi(m_2). \tag{23.107}$$

They satisfy the constraint

$$\tau^a \chi_a(m) = 0 \tag{23.108}$$

and the identities

$$i \epsilon_{abc} \tau^b \chi_c = \chi_a, \quad \tau^a \chi_b = -i \epsilon_{abc} \chi_c. \tag{23.109}$$

Inserting the matrix elements into the commutation relations (23.90) between nucleon and Δ-states, inserting a complete set of intermediate states, and using the covariant matrix elements (23.106) together with the completeness relations

$$\begin{aligned} \sum_m \chi_\alpha(m) \chi_\beta^*(m) &= \delta_{\alpha\beta},, \\ \sum_m \chi_a(m) \chi_b^*(m) &= \frac{2}{3} \delta_{ab} - \frac{1}{6} [\tau^a, \tau^a], \end{aligned} \tag{23.110}$$

we find once more the sum rules (23.98), (23.102), (23.104).

So far, these relations hold for the $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ subgroup of $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$. Extending the procedure from SU(2) to SU(3), we decompose the irreducible matrix of Q_5^3 between protons, remembering (23.65), as

$$G_A = F + D, \tag{23.111}$$

and consider once more the same commutators (23.91) between Σ^+ states, giving

$$|\langle \Sigma^0 | Q_5^- | \Sigma^+ \rangle|^2 + |\langle \Lambda | Q_5^- | \Sigma^+ \rangle|^2 + |\langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle|^2 = 2, \tag{23.112}$$

where Σ^{*0} is the strange partner of the Δ^0 resonance. The matrix element Q_5^3 between two Σ^+ states is, using the SU(3) decomposition as in Eq. (23.64),

$$\langle \Sigma^+ | Q_5^0 | \Sigma^+ \rangle = F. \tag{23.113}$$

Hence, by the Wigner-Eckart theorem for the SU(2) subgroup,

$$\langle \Sigma^0 | Q_5^- | \Sigma^+ \rangle = \sqrt{2} F. \tag{23.114}$$

Using once more the SU(3) decomposition (23.64), we calculate the matrix element

$$\begin{aligned} \langle \Lambda^0 | Q_5^- | \Sigma^+ \rangle &= F \cdot \left(-i f_{1-i2,8,(1+i2)/\sqrt{2}} \right) + D \cdot d_{1-i2,8,(1+i2)/\sqrt{2}} \\ &= D\sqrt{2} d_{118} = \sqrt{\frac{2}{3}} D. \end{aligned} \tag{23.115}$$

Similarly, the matrix element of

$$\langle \Delta^0 | Q_5^- | p \rangle = \frac{1}{\sqrt{2}} G^* \tag{23.116}$$

is related to $\langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle$ by SU(3) symmetry. Using the Clebsch-Gordan coefficients of the Particle Data Table we have

$$\begin{aligned} \langle \Delta^0 | Q_5^- | p \rangle &= -\langle \tfrac{3}{2}, -\tfrac{1}{2} | 1, -1; \tfrac{1}{2}, \tfrac{1}{2} \rangle \left(-\sqrt{\frac{1}{2}} \right) a, \\ \langle \Sigma^0 | Q_5^- | \Sigma^+ \rangle &= -\langle 1, 0 | 1, -1; 1, 1 \rangle \\ &= -\frac{1}{\sqrt{2}} \sqrt{\frac{2}{12}} a = \frac{1}{3\sqrt{2}} a, \end{aligned} \tag{23.117}$$

where a is some number. Using these equations we find from (23.116)

$$\langle \Sigma^{*0} | Q_5^- | \Sigma^+ \rangle = -\frac{1}{2} G^*. \tag{23.118}$$

The sum rule (23.112) becomes therefore

$$F^2 + \frac{1}{3} D^2 + \frac{1}{8} G^{*2} = 1. \tag{23.119}$$

Given the solution of the $\mathrm{SU}(2)_L + \mathrm{SU}(2)_R$ algebra (23.105), we find from this additional relation the F/D ratio $\frac{2}{3}$.

For completeness, let us also look at the commutation rule (23.91) between Ξ^+ particles, which gives the sum rule

$$|\langle\Xi^0|Q_5^-|\Xi^+\rangle|^2 + |\langle\Xi^{*0}|Q_5^-|\Xi^+\rangle|^2 = 1. \tag{23.120}$$

Within SU(3), Ξ^+, Ξ^0 have the vector indices $6 - i7/\sqrt{2}$ and $4 - i5/\sqrt{2}$ so that the decomposition (23.64) reads

$$\begin{aligned} \langle\Xi^-|Q_5^-|\Xi^+\rangle &= F\cdot(-if_{1-i2,(4+i5)/\sqrt{2},-(6-i7)/\sqrt{2}}) + D\cdot d_{1-i2,(4+i5)/\sqrt{2},-(6-i7)/\sqrt{2}} \\ &= F\cdot 2f_{147} + D\cdot(-2d_{146}) \\ &= F - D. \end{aligned} \tag{23.121}$$

The matrix element between $\Xi^{*0}(1530)$ and Ξ^+, on the other hand, has the SU(3) irreducible matrix elements

$$\begin{aligned} \langle\Xi^{*0}|Q^-|\Xi^+\rangle &= \sqrt{2}\langle\tfrac{1}{2},-\tfrac{1}{2}|1,-1;\tfrac{1}{2},\frac{1}{2}\rangle\tfrac{1}{2}a \\ &= \sqrt{2}\left(-\sqrt{\frac{2}{3}}\right)\frac{1}{2}a, \end{aligned} \tag{23.122}$$

to be compared with

$$\begin{aligned} \langle\Delta^0|Q_5^-|p\rangle &= \sqrt{2}\langle\tfrac{3}{2},-\tfrac{1}{2}|1,-1;\tfrac{1}{2},\tfrac{1}{2}\rangle\left(-\frac{1}{\sqrt{2}}\right)a \\ &= \sqrt{2}\frac{1}{\sqrt{3}}\left(-\frac{1}{\sqrt{2}}\right)a. \end{aligned} \tag{23.123}$$

Hence

$$\langle\Xi^{*0}|Q_5^-|\Xi^+\rangle = \frac{1}{\sqrt{2}}G^*, \tag{23.124}$$

and the sum rule reads

$$(F-D)^2 + \frac{1}{2}G^{*2} = 1. \tag{23.125}$$

It is satisfied by

$$F = \frac{2}{3}, D = \frac{1}{3}, G^* = \frac{4}{3}. \tag{23.126}$$

23.4 Supersymmetry

In 1974,[6] a new type of symmetry was discovered which extended the Poincaré group in a nontrivial way. It allowed for irreducible multiplets which contain simultaneously fermions and bosons. The basic example is given by the free action

$$\mathcal{A} = \int d^4x \left[\frac{1}{2}(\partial A)^2 + \frac{1}{2}(\partial B)^2 + \frac{1}{2}F^2 + \frac{1}{2}G^2 + M(FA + GB)\right)$$

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[6] Akulov and Volkov, ?????????? J. Wess and B. Zumino, Phys. Lett. B *49*, 521 (1974), B *59*, 163 (1975), Nucl. Phys. B *70*, 39, 1974, B *76*, 310, B *78*, 1 , 1974.

$$+\frac{1}{2}\left(\bar{\chi}\not\partial\chi - M\right)\bar{\chi}\chi)\Big] \tag{23.127}$$

where A, B, C, D are four real scalar fields and χ is a four component real Majorana spinor. The four scalar fields can be transformed into the four components of the Majorana field by the following transformations

$$\begin{aligned} \delta\chi &= [F + i\gamma_5 6 - i\not\partial\,(A + i\gamma_5 B)]\,\epsilon, \\ \delta\bar{\chi} &= \bar{\epsilon}[F + i\gamma_5 G + i(A + i\gamma_5 B)\,\overleftarrow{\not\partial}], \end{aligned} \tag{23.128}$$

$$\begin{aligned} \delta A &= \bar{\epsilon}\chi, & \delta F &= \bar{\epsilon}(-i\not\partial\,\chi), \\ \delta B &= \bar{\epsilon} i\gamma_5\chi, & \delta G &= \bar{\epsilon}[-i\not\partial\,(-i\gamma_5)]\chi. \end{aligned} \tag{23.129}$$

Here ϵ is a four-component real parameter with spinor indices. The spinor character makes it necessary to require ϵ and χ to be Grassmann variables which anticommute with each other

$$\epsilon_\alpha\chi_\beta = -\chi_\beta\epsilon_\alpha. \tag{23.130}$$

It is easy to verify that these transformations leave the action invariant. For the mass terms we calculate,

$$\delta(FA) = \bar{\epsilon}(-i\not\partial\,\chi)A + F\bar{\epsilon}\chi, \tag{23.131}$$

$$\delta(CB) = \bar{\epsilon}[-i\not\partial\,(-i\gamma_5)\chi]B + G\bar{\epsilon}i\gamma_5\chi \tag{23.132}$$

$$\begin{aligned} \frac{1}{2}\delta|\bar{\chi}\chi| &= \frac{1}{2}\bar{\chi}[F + i\gamma_5 G - i\not\partial\,(A + i\gamma_5 B)]\epsilon \\ &\quad + \frac{1}{2}\bar{\epsilon}[F + i\gamma_5 G + i(A + i\gamma_5 B)\,\overleftarrow{\not\partial}]\chi. \end{aligned} \tag{23.133}$$

Since a real spinor satisfies

$$\bar{\chi}^T = \gamma_0\chi = C\chi = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}\chi, \tag{23.134}$$

we see that

$$\begin{aligned} \bar{\chi}\epsilon &= \chi^T\gamma_0^T\epsilon = -\epsilon^T\gamma_0\chi = \epsilon^T\gamma_0^T\chi = \bar{\epsilon}\chi, \\ \bar{\chi}\gamma_5\epsilon &= \chi^T\gamma_0^T\gamma_5\gamma_0\bar{\epsilon}^T = \chi^T\gamma_5\epsilon^T = -\bar{\epsilon}\gamma_5^T\chi = \bar{\epsilon}\gamma_5\chi. \end{aligned} \tag{23.135}$$

Recall that in the Majorana representation

$$\gamma_5 = \begin{pmatrix} \boldsymbol{\sigma}^2 & 0 \\ 0 & -\boldsymbol{\sigma}^2 \end{pmatrix}$$

so that $\gamma_5^T = -\gamma_5$.
Hence the F and G terms in the transformation (23.133) are

$$\frac{1}{2}\delta(\bar{\chi}\chi) = \bar{\epsilon}(F + i\gamma_5 G)\chi, \tag{23.136}$$

and cancel in the transformation of the total mass term

$$FA + GB - \frac{1}{2}\bar{\chi}\chi.$$

What about the A, B terms. We write these terms in (23.133) as

$$\begin{aligned} \frac{1}{2}\delta(\bar{\chi}\chi) &= \frac{1}{2}\partial^{\mu}\left\{\bar{\chi}[-i\gamma_{\mu}(A + i\gamma_5 B)]\epsilon + \bar{\epsilon}i(A + i\gamma_5 B)\gamma_{\mu}\chi\right\} \\ & - \left\{-\frac{1}{2}\bar{\chi}\overset{\leftarrow}{\not\partial}(A + i\gamma_5 B)\epsilon - \frac{1}{2}\bar{\epsilon}i(A + i\gamma_5 B)\chi\right\}. \end{aligned} \qquad (23.137)$$

The first term is a pure surface term and does not contribute to the total action. In the third we use

$$\begin{aligned} \bar{\chi}\gamma_{\mu}\epsilon &= -\bar{\epsilon}\gamma_{\mu}\chi, \\ \bar{\chi}\gamma_{\mu}\gamma_5\epsilon &= -\bar{\epsilon}\gamma_5\gamma_{\mu}\chi, \end{aligned} \qquad (23.138)$$

and see that it is equal to the forth term. Both together cancel the FG terms in $\delta(FA + GB)$. Thus the total action is invariant. The transformations are called *supersymmetry transformation* and the action *supersymmetric.*

Notice that the fields F, G are not dynamical since they carry no gradients in the action. They could be eliminated from the action using the equations of motion but then the verification of the supersymmetry would be much more involved. For this they are essential since only with them the four components of χ have four real counterparts A, B, G, F. In a free field theory, the equations of motion make F, G vanish. When interactions are included, they are still non-dynamical but no longer zero.

In particles physics, no indication of some broken supersymmetry have been discovered so far. There exists, however, a supersymmetry between the unphysical content in gauge fields and the Fadeev-Popov ghost fields in QED, which were needed to remove the vacuum energy of the two unphysical modes. Recall the Lagrangian (5.510):

$$\mathcal{L}_{\rm tot} = \mathcal{L} + \mathcal{L}_{\rm GF} + \mathcal{L}_{\rm ghost} = -\frac{1}{4}F_{\mu\nu}{}^2 - D(x)\partial^{\mu}A_{\mu}(x) + \alpha D^2(x)/2 - i\partial_{\mu}\bar{C}\partial^{\mu}C. \qquad (23.139)$$

It is is invariant under the following two sets of supersymmetry transformations:

$$\begin{aligned} \delta A_{\mu} &= i\partial_{\mu}C, \\ \delta\bar{C} &= D, \\ \delta C &= \delta D = 0, \end{aligned} \qquad (23.140)$$

and

$$\begin{aligned} \bar{\delta}A_{\mu} &= i\partial_{\mu}\bar{C}, \\ \bar{\delta}C &= -D, \\ \bar{\delta}\bar{C} &= \bar{\delta}D = 0. \end{aligned} \qquad (23.141)$$

These are known as the BRS transformations (see Footnote 8 in Chapter 4).

The BRS symmetry is generates by charges

$$
\begin{aligned}
Q &= \sum_{\mathbf{k}} \omega_{\mathbf{k}}(a_{\mathbf{k},l} c_{\mathbf{k}} + \text{h.c.}), \\
\bar{Q} &= \sum_{\mathbf{k}} \omega_{\mathbf{k}}(a_{\mathbf{k},l} \bar{c}_{\mathbf{k}} + \text{h.c.}).
\end{aligned}
\tag{23.142}
$$

Together with the subsidiary conditions (5.508), the conditions

$$
Q|0\rangle = 0, \qquad , \bar{Q}|0\rangle = 0 \tag{23.143}
$$

are seen to enforce precisely the Gupta-Bleuler subsidiary condition (5.487).[7]

Note that by postulating the absence of ghosts from the Hilbert space at a specific time, they are excluded for all times since the Lagrangian preserves ghost charge. This a consequance of the invaraice

$$
C \to e^{\alpha} C, \qquad \bar{C} \to e^{-\alpha} \bar{C}. \tag{23.144}
$$

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[7] For details see T. Kugo and I. Ojima, Suppl. Prog. Theor. Phys. *66*, 1 (1979). J. Ambjorn and R.J. Hughes, Nucl. Phys. B *217*, 336 (1983).

24

Quantum Field Theoryof Elementary Particles

The quantum field-theoretic description of electromagnetic interactions in Chapter 10 is able to explain and predict experimental data, with extreme accuracy, over a wide range of phenomena involving electrons and photons. The question arises whether one can find similar quantum field theories for other interactions. These are classified according to their strength as gravitational, weak, or strong. The interaction strength of these are so widely different from each other, and from the electromagnetic strenght, that until the sixties of the ninetennth century, they required a separate description. If two particles are far apart from each other, only gravitational and electromagnetic interactions are present. If particles become very large, the gravitational interactions become dominant. The dimensionless constant characterizing the strength of the electromagnetic interactions is the fine-structure constant (recall Footnote ?? on p. ??)

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.035\,997\,9(3\,2)} = 7.297\,352\,63(25) \times 10^{-3}. \tag{24.1}$$

An analogous gravitational strength parameter is

$$\alpha_{\rm grav} = G\frac{M_p^2}{\hbar c} = 5.902(4) \times 10^{-39}. \tag{24.2}$$

The ratio between the two is of the order of 10^{-36}. Since this is extremely small, gravitational forces are relevant only for electrically neutral celestial bodies. [1]

If particles move close to each other, then strong and weak forces become active. The strong interations are characterized by coupling strengths of the order of unity, for instance between nucleons and pions:

$$\alpha_{\rm strong} = \frac{g_{\pi NN}}{4\pi} = 14.4 \pm 0.4 \tag{24.3}$$

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[1] Note that if the charges of electrons and protons would not be precisely euqal, a study of the motion of planets could require including Coulomb forces.

The dimensionless constant governing weak forces, to be studied in detail later, can be introduced as a *weak fine-structure constant*

$$\alpha_{\rm weak} = g\frac{M_p^2 c}{\hbar^3} = 1.0121(3) \times 10^{-5}. \tag{24.4}$$

Its strength lies between the first two.

Just as electromagnetic, the weak interactions can be dealt with efficiently and accurately by quantum field theory. Due to the weakness of the interactions, lowest order prturbation theory is sufficient for any process to be studied. The same thing is true for gravitational interactions at long distances. However, at short distances of the order of the Planck length

$$L_p = \frac{\hbar}{M_p c} \approx 1.617 \times 10^{-33}{\rm cm}, \tag{24.5}$$

the zero-point quantum fluctuations of the gravitational field pose serious problems and the theory cannot, as yet, be extended to this regime.

In the last 15 years, many attempts have been made to unify all these interactions in a single field theory. For electromagnetism and weak interactions, a consistent unification has been found by Glashow, Weinberg, and Salam, now often called the standard model of *electroweak interactions*. For the other interactions, we have to wait for the future developments.

24.1 Electromagnetism

The best understood interaction, the electromagnetic one of electrons, has been described in detail in Chapter 10. It emerged straight-forwardly from Maxwell's theory, where the interaction is

$$\mathcal{A}_{\rm int} = \int d^4x \mathcal{L}_{\rm int}(x) = \int d^4x j^\mu(x) A_\mu(x) \tag{24.6}$$

with $j^\mu(x)$being is the total local conserved current density of all charged particles. In field theory, this becomes the total Noether current of all complex fields following from the invariance of their actions under global chages of their phase [global $U(1)$-invariance]. This current obeys the local conservation law

$$\partial_\mu j^\mu(x) = 0. \tag{24.7}$$

This guarantees the invariance of the interaction with respect to arbitrary local gauge transformations

$$A_\mu(x) \to A_\mu(x) + \partial_\mu \Lambda(x). \tag{24.8}$$

In Chapter 10 we have seen that the coupling (24.6) can be thought of as arising from a simple modification of the derivative parts of the action. Each derivative has to be replaced by the covariant derivative (minimal substitution) (see p. 559).

For a charged scalar field of charge e, this replacement produces more than a linear interaction with the vector potential. a term quadratic in A_μ. The minimal gauge-invariant extension of the interaction (24.6) leads to the total action

$$\begin{aligned} \mathcal{A} &= \mathcal{A}_\gamma + \mathcal{A}_\varphi + \mathcal{A}_{\text{int}} \\ &= \int d^4x \left[-\frac{1}{4} {F_{\mu\nu}}^2 + \frac{1}{2} |(\partial_\mu - ieA_\mu)\varphi|^2 + \frac{M^2}{2} |\varphi|^2 \right]. \end{aligned} \tag{24.9}$$

The minimal substitution

$$\partial_\mu \to D_\mu \equiv \partial_\mu + ieA_\mu \tag{24.10}$$

is of course the quantum-mechanical analog of the momentum replacement

$$p_\mu \to P_\mu \; = \; p_\mu - eA_\mu. \tag{24.11}$$

To make the action (24.9) gauge invariant, the gauge transformations of the vector potential

$$A_\mu(x) \to A_\mu(x) + \partial_\mu \Lambda(x) \tag{24.12}$$

must be accompanied by a local U(1) phase transformation of the complex scalar fields

$$\varphi(x) \to e^{-ie\Lambda(x)} \varphi(x). \tag{24.13}$$

In contrast to the ordinary derivative $\partial_\mu \varphi(x)$, the quantity $D_\mu \varphi(x)$ behaves under spacetime-dependent U(1) transformations just like the field $\varphi(x)$ itself:

$$D\varphi(x) \to e^{-ie\Lambda(x)} D\varphi(x). \tag{24.14}$$

This is why it is called the *covariant derivative* (see p. 561).

Compare (24.9) with the action of a Dirac particle of charge e, which reads

$$H \; = \; \mathcal{A}_\gamma + A_\psi + \mathcal{A}_{\text{int}} \tag{24.15}$$

$$\; = \; \int d^4x \left(-\frac{1}{4} {F_{\mu\nu}}^2 + \bar\psi i \not{D} \psi - m\bar\psi\psi \right). \tag{24.16}$$

In contrast to (24.9), this is linear in A_μ and no A^2-term is necessary to ensure the invariance under the local gauge transformations

$$\begin{aligned} A_\mu &\to A_\mu + \partial_\mu \Lambda \\ \psi &\to e^{-ie\Lambda(x)} \psi. \end{aligned} \tag{24.17}$$

For electrons and other charged leptons such as μ and τ, the charge is $e = -\sqrt{4\pi\alpha}$, where $\alpha \approx 1/137$ is the fine-structure constant (24.1).

24.2 Gravity

The gravitational interaction between static point masses at a long distance has been known since Newton. It depends only on the size of the masses. In terms of the spin 2 tensor fields whose free-field behavior was discussed in Chapter 4, it reads, in analogy with the very similar looking (24.6),

$$\mathcal{A}_{\rm int} = \int dx\, \mathcal{L}_{\rm int}(x) = -\frac{1}{2}\int d^4x\, h^{\mu\nu}(x) T_{\mu\nu}(x) \tag{24.18}$$

where $T_{\mu\nu}(x)$ is the symmetric energy momentum tensor of the entire matter distribution in space. For a single classical point particle moving along some trajectory $x^\mu(t)$ with a four-momentum $p^\mu(t)$ it reads

$$T_{\mu\nu}(x) = \frac{p_\mu(t)p_\nu(t)}{E}\delta^{(3)}(\mathbf{x}-\mathbf{x}(t)). \tag{24.19}$$

The conservation law $\partial_\mu T^{\mu\nu}(x) = 0$ guarantees the invariance of the interaction under the local gauge transformations

$$h_{\mu\nu}(x) \rightarrow h_{\mu\nu}(x) + \partial^\mu \Lambda^\nu(x) + \partial^\nu \Lambda^\mu(x). \tag{24.20}$$

For a particle of mass M lying at the rest of the coordinate origin, the only non-zero component is

$$T_{00} = M\delta^{(3)}(\mathbf{x}). \tag{24.21}$$

The gravitational field in the presence of a non-zero $T_{\mu\nu}(x)$ satisfies the field equation

$$-\frac{1}{2}\partial^2 \phi^{\mu\nu}(x) = c\kappa T^{\mu\nu}(x), \tag{24.22}$$

where [recall (5.609)]

$$\phi^{\mu\nu} = h^{\mu\nu} - \frac{1}{2}g^{\mu\nu}h.$$

The equation is solved with the help of the retarded Green function (5.179) as in (5.180) (5.182), yielding

$$\begin{aligned}\phi^{\mu\nu}(x) &= 2c\kappa\frac{1}{i}\int G_R(x,x')T^{\mu\nu}(x') \\ &= -2c\kappa\int d^3x' \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}T^{\mu\nu}(t_R,\mathbf{x}'),\end{aligned} \tag{24.23}$$

For the particle at the origin, the only non-vanishing field component is

$$\phi^{00}(x) = -2c\kappa M\frac{2c\kappa M}{4\pi|\mathbf{x}|}. \tag{24.24}$$

If the mass point moves slowly along the trajectory $\bar{\mathbf{x}}(t)$, the field tensor components $\phi^{0i}(x)$ and $\phi^{ij}(x)$ are strongly supressed by factors $\dot{\bar{\mathbf{x}}}/c$. The leading component $\phi^{00}(t, \mathbf{x})$ is given by an equation like (5A.8):

$$\phi^{00}(t, \mathbf{x}) = -\frac{2c\kappa M}{4\pi r_{\mathrm{ret}}(t)} \tag{24.25}$$

where

$$r_{\mathrm{ret}}(t) = |\mathbf{x} - \bar{\mathbf{x}}(t_R)| \tag{24.26}$$

is the retarded distance of the point $\mathbf{x}$ from the source [see (5A.9)].

The deviation $h_{\mu\nu}$ of the metric $g_{\mu\nu}$ from the flat Minkowski metric has the nonzero field components

$$h_{00} = h_{ii} = \frac{1}{2}\phi_{00}. \tag{24.27}$$

When inserted back into the interaction (24.18), the field $h^{\mu\nu}(x)$ leads to an interaction energy at a distance r between two masses

$$E_{\mathrm{int}} = \frac{c\kappa M M'}{8\pi r_{\mathrm{ret}}}. \tag{24.28}$$

This corresponds to Newton's law with the gravitational constant

$$G = \frac{c\kappa}{8\pi} = 6.67 \times 10^{-8}\mathrm{cm}^{-3}\mathrm{s}^{-2}\mathrm{g}^{-1}. \tag{24.29}$$

24.3 Strong Interactions

Elementary particles which interact strongly with each other are called *hadrons*. According to their statistics, one distinguishes *baryons* and *mesons*. The most prominent spin-1/2 particles in nuclear matter, protons and neutrons, are baryons. The forces between these arise, to lowest approximation, from the existence of a spin-0 meson called pion. The names baryons (heavy particles) and mesons (middle-heavy particles) indicate that the initially known baryons were the heaviest elementary particles, the mesons were in mass between the baryons and the leptons.

Hadrons exhibit rich spectra as we have seen in Chapters 22 and 23). Approximately, these were explained by *quark models*. Just as nuclei are composed of protons and neutrons, baryons are bound states of three quarks, mesons of a quark and an antiquark.

In spite of its successes, the quark model exhibited several fundamental inconsistencies. Most importantly: For any reasonable potential between quarks, the ground state orbital wave function should always be without zeros implying vanishing relative angular momenta for each pair of quarks. Any higher angular momentum would have at least one zero in the wave function which would increase the gradient (=kinetic) energy of the Schrödinger field via the centreifugal barrier. The orbital wave function of the ground state of three quarks, the proton, must therefore be symmetric under the exchange of two quarks. On the other hand, the SU(6) wave function involving internal SU(3) and spin has the Yang tableau $\square\square\square$. But this implies that the nucleon wave function is completely symmetric under exchange of all positions, all SU(3), and all spin variables. This seems to contardict the fact that quarks have spin 1/2 so that, by the spin statistics theorem, they should be fermions and therefore have a completely antisymmetric wave function.

To remedy this contradiction, Han and Nambu suggested that quarks should be triplet under a further SU(3) group of transformations now called color SU(3).[2] Color appears as a further label to the quark fields

$$q(x) = \begin{pmatrix} u(x) \\ d(x) \\ s(x) \\ c(x) \end{pmatrix}$$

which should be written as

$$q_\alpha(x) = \begin{pmatrix} u_\alpha(x) \\ d_\alpha(x) \\ s_\alpha(x) \\ c_\alpha(x) \end{pmatrix}.$$

By postulating that all hadron states are completely antisymmetric in color, i.e. color singlets, the contadictions disappears and the spin statistic relation is again valid.

After this somewhat artificial postulate the question arose how nature manages to enforce the color antisymmetry, i.e., how it prevents color non-singlet states to be excited. The answer suggested by Fritzsch and Gell-Mann was that color SU(3) was a local gauge symmetry of hadronic physics. The action had to be invariant under arbitrary non-abelian SU(3)-transformations of the quark fields

$$q(x) \rightarrow e^{-i\alpha^a(x)\lambda^a/2} q(x), \tag{24.30}$$

where the matrices λ^a now act on the three color SU(3) of the quark $q(x)$.

The tripling of the quarks saved not only the validity of the spin statistics relation for quarks. Also the particle decay

$$\pi^0 \rightarrow \gamma\gamma$$

which is observed experimentally at a rate $\Gamma = 8.4 \times 10^{-17}$s. Also the total interaction cross section observed in $e^+ \, e^-$ collisions could only be explained if the each quark occured in three colored versions.

Once it was postulated that the quark action be invariant under local symmetry transformations, it became necessary to introduce a gauge field to maintain the invariance of the gradient term in the action. This led to the quark Lagrangian

$$\mathcal{L}(x) = \bar{q}(x) i \not{D} \, q(x) - M \bar{q}(x) q(x) \tag{24.31}$$

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[2] H. Fritzsch, M. Gell-Mann, Intern. conf. on Duality and Symmetry in Hadron Physics, Weizmann Science Press, 1971; H. Fritzsch, M. Gell-Mann, H. Leutwyler, Phys. Lett. B *47*, 365 (1973).

where $q(x)$ carries flavor indices distinguishing the quarks $u, d, c, s, \ldots$ and three color indices. The gradient term contains the covariant derivative

$$\not{D} = \gamma^\mu D_\mu = \gamma^\mu \left(\partial_\mu + igA_\mu\right) \tag{24.32}$$

where A_μ is a 3×3 matrix in color space to guarantee that D_μ transforms under local color SU(3) transformations in the same way as the field $\psi(x)$ itself [compare (24.14)]

$$D_\mu q(x) \rightarrow U(x) D_\mu q(x) = e^{-i\alpha_a(x)\lambda^a/2} D_\mu q(x). \tag{24.33}$$

The covariance property is a bit harder to show than for electromagnetism. The derivative of the field goes over into:

$$\begin{aligned} \partial_\mu q(x) &\rightarrow \partial_\mu U(x) q(x) = U(x)[U^{-1}(x)\partial_\mu U(x) q(x)] \\ &= U(x)\partial_\mu q(x) + U(x)[U^{-1}(x)\partial_\mu U(x)] q(x). \end{aligned} \tag{24.34}$$

In order to remove the second term, the gauge field A_μ has to transform like

$$A_\mu(x) \rightarrow U(x) A_\mu(x) U^{-1}(x) - \frac{1}{ig}[\partial_\mu U(x)] U^{-1}(x) \tag{24.35}$$

$$= U(x) A_\mu(x) U^{-1}(x) + \frac{1}{ig} U(x) \partial_\mu U^{-1}(x). \tag{24.36}$$

Then

$$\begin{aligned} \left[\partial_\mu + igA_\mu(x)\right] q(x) &\rightarrow U(x)\left[\partial_\mu + iqA_\mu(x) + U^\dagger(x)\partial_\mu U(x)\right] \\ &= U(x)\left[\partial_\mu + igA_\mu(x)\right] q(x). \end{aligned} \tag{24.37}$$

which is the desired covariant transformation law.

After the introduction of such a gauge field, an interaction has to be found describing the dynamics of this gauge field itself. If color is never to be observed, the action of the gauge field should be locally SU(3) invariant as well. The only Lagrangian which has this property and contains of most first derivatives in A_μ is given by

$$\mathcal{L}_{\text{gluon}} = -\frac{1}{2}\text{tr}\left(G_{\mu\nu} G^{\mu\nu}\right) \tag{24.38}$$

where

$$G_{\mu\nu} = \partial_\mu A_\mu - \partial_\nu A_\mu + ig[A_\mu, A_\nu] \tag{24.39}$$

is the field tensor, the covariant curl of the vector potential A_μ. Just as A_μ, the field tensor is a 3×3 matrix in color space. It is easy to verify that the matrix $G_{\mu\nu}$ transforms under SU(3) covariantly as follows

$$G_{\mu\nu}(x) \rightarrow U(x) G_{\mu\nu}(x) U(x). \tag{24.40}$$

The theory is described by the Lagrangian

$$\mathcal{L}(x)=\bar{q}(x)i\left[\partial_\mu+igA_\mu(x)\right]q(x)-\frac{1}{2}\mathrm{tr}\left[G_{\mu\nu}(x)G^{\mu\nu}(x)\right]. \tag{24.41}$$

This Lagrangian is a complete nonabelian analog of the gauge field Lagrangian (10.1) (10.3) of quantum electrodynamics (QED). For this reason it has been given the similar name *quantumchromodynamics* (QCD).

Instead of 3×3 matrices A_μ, $G_{\mu\nu}$, one can also use an octet of vector and tensor fields defined by

$$\begin{aligned}A_\mu &= \frac{\lambda^a}{2}A_\mu{}^a\\ G_{\mu\nu} &= \frac{\lambda^a}{2}G^a_{\mu\nu}.\end{aligned} \tag{24.42}$$

Thus we can write the Lagrangian of QCD as

$$\mathcal{L}=\bar{q}(x)i\gamma^\mu\left[\partial_\mu+ig\frac{\lambda^a}{2}A^a_\mu(x)\right]q(x)-\frac{1}{4}G^a_{\mu\nu}(x)G^a_{\mu\nu}(x), \tag{24.43}$$

where

$$G^a_{\mu\nu}(x)=\partial_\mu A^a_\nu(x)-\partial_\nu A^a_\mu(x)-q\epsilon^{abc}A^b_\mu(x)A^c_\nu(x). \tag{24.44}$$

In the last twenty years, evidence has accumulated that the gauge field A^a_μ is indeed capable of describing the forces which bind together the quarks inside the hadrons. The field quanta carried by A^a_μ are called gluons. At first, the masses of the quarks are approximated to be equal to zero. The Lagrangian has an additional invariance. If the flavor group is taken to be SU(3), it is extended to SU(3) × SU(3), the chiral symmetry group of flavor. Its Noether current densities are

$$\begin{aligned}j^\mu_a(x) &= \bar{q}(x)\gamma^\mu\frac{\lambda_a}{2}q(x)\\ j^\mu_{5a}(x) &= \bar{q}(x)\gamma^\mu\gamma_5\frac{\lambda_a}{2}q(x),\end{aligned} \tag{24.45}$$

where the λ_a matrices act on the flavor SU(3) indices. The current densities are color singlets. The corresponding color octet currents are not observable, due to local SU(3) color invariance.

After field quantization the field components satisfy the local SU(3) × SU(3) commutation rules derived in (6.252) and discussed in Section 23.3. The charges Q_a and axial charges Q_{5a} defined by

$$\begin{aligned}Q_a &= \int d^3xj^0\\ Q_{5a} &= \int d^3xj^0_{5a}\end{aligned} \tag{24.46}$$

form the Lie algebra

$$\begin{aligned}
[Q_a, Q_b] &= i f_{abc} Q_c, && (24.47)\\
[Q_a, Q_{5b}] &= i f_{abc} Q_{5c}, && (24.48)\\
[Q_{5a}, Q_{5b}] &= i f_{abc} Q_c && (24.49)
\end{aligned}$$

and the chiral charges

$$Q_a^L = (Q_a - Q_{5a})/2, \qquad Q_a^R = (Q_a + Q_{5a})/2, \tag{24.50}$$

generate two commuting groups $\mathrm{SU}(3)_\mathrm{L}$ and $\mathrm{SU}(3)_\mathrm{R}$, respectively. Due to the chiral invariance of the massless quark gluon Lagrangian (24.43), the currents are conserved.

$$\begin{aligned}
\partial_\mu j^\mu(x) &= 0,\\
\partial_\mu j_5^\mu(x) &= 0. && (24.51)
\end{aligned}$$

The ground state of the theory breaks the axial part of this symmetry spontaneously. this gives rise to non-zero quark masses. The spontaneous breakdown is accompanied by massless pseudoscalar Nambu-Goldstone bosons, which are identified with the pion and its flavor octet partners.

In nature, quarks are not massless and the axial charge are not conserved. The masses of non-strange quarks are, however, very small so that the axial charges with the SU(2)-indices $a = 1, 2$ are approximately conserved. This is the basis of the PCAC hypothesis (partial conservation of axial vector current). The masses for $m_u, m_d, m_s \ldots$ raises the mass of the pion and the other pseudoscalar mesons to the to the experimental nonzero values. The quark masses which give a consistent picture of experimantal data are[3]

$$\begin{pmatrix} m_u \\ m_d \\ m_s \\ m_c \\ m_t \\ m_b \end{pmatrix} = \begin{pmatrix} 4.5 \pm 1.4 \\ 7.9 \pm 2.4 \\ 155 \pm 50 \\ 1270 \pm 50 \\ 40000 \pm 10000 \\ 4250 \pm \pm 100 \end{pmatrix} \mathrm{MeV}. \tag{24.52}$$

In recent years, much insight into the theory has been gained from computer simulations of lattice models of the theory. They have continued that the theory has the desired properties to explain the many strongly interacting particles observed in the laboratory.

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[3] See J. Gasser and H. Leutwyler, Phys. Rep. *87*, 77 (1982); G. Harrison et al. Phys. Lett. B *47*, 493 (1984).

24.4 Weak Interactions

The decay of nuclei proceeds via α, β, γ radiation or by fission. The first process is governed by nuclear forces, the third by electromagnetic forces. The β-decay has an entirely different origin. Initially, it posed the puzzle that the emerging particles, which are electrons or positrons, did not come out with a fixed energy which should be equal to the mass difference between initial and final nuclei. Instead, they had an energy distribution with a maximal energy at the correct value. This led Nils Bohr had to speculate that energy conservation could possibly be violated in quantum physics. In a historic letter written 1930 to colleagues at a meeting in Tübingen, however, Wolfgang Pauli suggested that the missing energy was carried off by a neutral particle, now called *neutrino*. Its spin had to be 1/2, to preserve angular momentum. The simplest nuclear particle which shows β-decay is the neutron itself which decays, after about 900 seconds, as follows

$$n \rightarrow p + e^- + \bar{\nu}_e \tag{24.53}$$

where $\bar{\nu}$ denotes a right-handed version of Pauli's particle which is nowadays called the antineutrino associated with the electron.

Fermi was the first to describe β-decay to lowest order in perturbation theory.[4] Initially he suggested a current-current coupling

$$\mathcal{L} = C\bar{p}(x)\gamma^\mu n(x)\bar{e}(x)\gamma_\mu \nu(x) + \text{c.c.}\ , \tag{24.54}$$

where we have used an obvious short notation for the fields: $\psi_e(x) \rightarrow e(x), \psi_p(x) \rightarrow p(x)$, etc.. This interaction looks like an electromagnetic one, except that the photon propagator which would cause a long-range interaction is replaced by a short-range δ-function interactions. Fermi also realized that for covariance reasons, there could be 5 such interactions

$$\begin{aligned} \mathcal{L} &= C_S\bar{p}(x)n(x)\bar{e}(x)\nu(x) + C_P\bar{p}(x)i\gamma_5 n(x)\bar{e}(x)i\gamma_5\nu(x) \\ &+ C_V \bar{p}(x)\gamma^\mu n(x)\bar{e}(x)\gamma_\mu\nu(x) + C_A\bar{p}(x)\gamma^\mu\gamma_5 n(x)\bar{e}(x)\gamma_\mu\gamma_5\nu(x) \\ &+ \tfrac{1}{2}C_T\bar{p}(x)\sigma^{\lambda\kappa}n(x)\bar{e}(x)\sigma_{\lambda\kappa}\nu(x) + \text{c.c.}\ . \end{aligned} \tag{24.55}$$

Requiring time reversal invariance (which is fulfilled to a great accuracy, so that its breakdown is observable only in very few distinguished processes), the coefficients C_i would have to be real. If Γ_i denotes the five Dirac matrices, we shall may write the interaction short as

$$\mathcal{L} = \sum_{i=S,P,V,A,T} \bar{p}(x)\Gamma_i n(x)\bar{e}(x)\Gamma_i\nu(x) + \text{c.c.}\ . \tag{24.56}$$

For a decay of an initial nucleus at rest $|\Psi_{\rm i}\rangle$ into a final nucleus $|\Psi_{\rm f}\rangle$, we have to evaluate the matrix elements

$$\langle\Psi_{\rm f}|\bar{p}(x)\Gamma_i n(x)|\Psi_{\rm i}\rangle. \tag{24.57}$$

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[4] E.Fermi, Nuovo Cimento *11*, 1 (1934); Z. Phys. *88*, 161 (1934).

Due to the small energies involved, the final state will also be at rest (if the nucleus is big enough), and we may use the nonrelatistic limit for the matrix elements between nucleons. Taking the Dirac matrices in Dirac's original representations, we can use the direct-product expressions (3.508) and rewrite the matrix elemsnts of $\bar{p}(x)\Gamma_i n(x)$ as follows:

$$\begin{array}{rl} S: & \bar{p}(x)n(x) \approx p^\dagger(x)n(x) \\ P: & \bar{p}(x)i\gamma^5 n(x) \approx -p^\dagger(x)\,\sigma^2 \times 1\, n(x) \approx 0 \\ V: & \bar{p}(x)\gamma^0 n(x) \approx p^\dagger(x)n(x) \\ & \bar{p}(x)\gamma^i n(x) \approx -p^\dagger(x)\,\sigma^1 \times \sigma^i\, n(x) \approx 0 \\ A: & \bar{p}(x)\gamma^0\gamma_5 n(x) \approx p^\dagger(x)\,\sigma^1 \times 1\, n(x) \approx 0 \\ & \bar{p}(x)\gamma^i\gamma_5 n(x) \approx p^\dagger(x)\,1 \times \sigma^i\, n(x) \\ T: & \bar{p}(x)\sigma^{0i} n(x) \approx -p^\dagger(x)\,\sigma^2 \times \sigma^i\, n(x) \approx 0 \\ & \bar{p}(x)\sigma^{ij} n(x) \approx \epsilon_{ijk}\, p^\dagger(x)\,1 \times \sigma^k\, n(x) \end{array} \tag{24.58}$$

The lines carrying a symbol ≈ 0. are ignored since they involve mixtures of upper and lower components. Thus we are left with only two types of nuclear matrix elements:

$$\begin{aligned} \langle \Psi_{\rm f}|p^\dagger(x)n(x)|\Psi_{\rm i}\rangle &\equiv \langle\, \mathbf{1}\,\rangle, \\ \langle \Psi_{\rm f}|p^\dagger(x)\,\boldsymbol{\sigma}\,n(x)|\Psi_{\rm i}\rangle &\equiv \langle\, \boldsymbol{\sigma}\,\rangle. \end{aligned} \tag{24.59}$$

The S-matrix elements are then approxiamtely given by

$$S = 1 - 2\pi i\delta(E_{\rm f} + E_e + E_{\bar\nu} - E_{\rm i})R, \tag{24.60}$$

with the R-matrix

$$\begin{aligned} R \;=\; & \frac{\sqrt{2m_\nu}}{V}\Big\{\langle\, \mathbf{1}\,\rangle \Big[C_S\bar{u}(\mathbf{p}_e)v(\mathbf{p}_{\bar\nu}) + C_V\bar{u}(\mathbf{p}_e)\gamma^0 v(\mathbf{p}_{\bar\nu})\Big] \\ & +\langle\, \boldsymbol{\sigma}\,\rangle \left[\tfrac{1}{2}C_T\bar{u}(\mathbf{p}_e)\boldsymbol{\sigma} v(\mathbf{p}_{\bar\nu}) + C_A\bar{u}(\mathbf{p}_e)\boldsymbol{\gamma}\gamma_5 v(\mathbf{p}_{\bar\nu})\right]\Big\}, \end{aligned} \tag{24.61}$$

where $\boldsymbol{\sigma}$ in front of a Dirac spinor means $1 \times \boldsymbol{\sigma}$. The spin labels s_3 for the electron and antineutrino have been omitted, for brevity. We have also normalized the antineutrino states in the same way as photon states like

$$\langle \mathbf{p}'_{\bar\nu}|\mathbf{p}_{\bar\nu}\rangle = 2p^0_{\bar\nu}\delta^{(3)}(\mathbf{p}'_{\bar\nu} - \mathbf{p}_{\bar\nu}) \tag{24.62}$$

to allow for a smooth limit $m_\nu \to 0$.

When calculating decay rates, we may sum over the antineutrino polarizations which are hard to measure. The polarization sum yields

$$\sqrt{2m_\nu}\sum_{\text{spin pol}} \bar{v}(\mathbf{p}_{\bar\nu})v(\mathbf{p}_{\bar\nu}) = \not{p}_{\bar\nu} - m_\nu, \tag{24.63}$$

and m_ν is set equal to zero et the end. For unpolarized nuclei, we have

$$\langle\, \sigma^i \sigma^j \,\rangle = \frac{1}{3}|\boldsymbol{\sigma}|^2, \qquad \langle\, \sigma^i \, \mathbf{1}\,\rangle = 0. \tag{24.64}$$

If also the electrons are unpolarized, we obtain

$$\begin{aligned}\sum_{\text{spin pol}} |R|^2 &= \frac{1}{2m_e V^2}\Big[C_S^2 |\langle \mathbf{1}\rangle|^2 \mathrm{tr}\,(\not p_{\bar\nu} \not p_e) + |C_V|^2 |\langle \mathbf{1}\rangle|^2 \mathrm{tr}\,(\gamma_0 \not p_{\bar\nu} \gamma_0 \not p_e) \\ &+ \tfrac{1}{3} C_A^2 |\langle \boldsymbol{\sigma}\rangle|^2 \mathrm{tr}\,(\gamma^i \gamma_5 \not p_{\bar\nu} \gamma_5 \gamma^i \not p_e) + \tfrac{1}{12} C_T^2 |\langle \boldsymbol{\sigma}\rangle|^2 \mathrm{tr}\,(\sigma^i \not p_{\bar\nu} \gamma_5 \sigma^i \not p_e) \\ &+ 2C_S C_V |\langle \mathbf{1}\rangle|^2 m_e \mathrm{tr}\,(\not p_{\bar\nu} \gamma_0) + \tfrac{1}{3} C_S C_V |\langle \boldsymbol{\sigma}\rangle|^2 m_e \mathrm{tr}\,(\sigma^i \not p_{\bar\nu} \gamma_0 \not p_e)\Big], \end{aligned} \tag{24.65}$$

or more explicitly

$$\begin{aligned}\sum_{\text{spin pol}} |R|^2 &= \frac{4E_\nu E_{\bar\nu}}{2m_e V^2}\left[C_S^2 |\langle \mathbf{1}\rangle|^2 \left(1 - \frac{\mathbf{p}_e \mathbf{p}_{\bar\nu}}{E_e E_{\bar\nu}}\right) + |C_V|^2 |\langle \mathbf{1}\rangle|^2 \left(1 + \frac{\mathbf{p}_e \mathbf{p}_{\bar\nu}}{E_e E_{\bar\nu}}\right)\right. \\ &\quad + C_A^2 |\langle \boldsymbol{\sigma}\rangle|^2 \left(1 - \frac{1}{3}\frac{\mathbf{p}_e \mathbf{p}_{\bar\nu}}{E_e E_{\bar\nu}}\right) + \frac{1}{4} C_T^2 |\langle \boldsymbol{\sigma}\rangle|^2 \left(1 + \frac{1}{3}\frac{\mathbf{p}_e \mathbf{p}_{\bar\nu}}{E_e E_{\bar\nu}}\right) \\ &\quad \left. + 2C_S C_V |\langle \mathbf{1}\rangle|^2 m_e \frac{2m_e}{E_e} - C_A C_T |\langle \boldsymbol{\sigma}\rangle|^2 \frac{m_e}{E_e}\right], \end{aligned} \tag{24.66}$$

The interference terms $C_S C_V$ and $C_T C_A$ show a strong threshold dependence proportional to $1/E_e$. Since this is not seen experimentally one must have

$$C_S C_V \approx 0, \qquad C_T C_A \approx 0. \tag{24.67}$$

One distinguishes now *Gamow-Teller transitions* for which $|\langle \boldsymbol{\sigma}\rangle|^2 \neq 0$, and *Fermi transitions* for which $|\langle \mathbf{1}\rangle|^2 \neq 0$ (both without nuclar parity change). For transitions in which initial and final nuclear spins are the same, only C_S^2 and C_V^2 contribute. These are distinguishable by the electronic-antineutrino correlation in momentum space. In the first case, electron and antineutrino come out preferably in opposite direction ($\mathbf{p}_e \mathbf{p}_{\bar\nu} < 0$), in the second case in the same direction ($\mathbf{p}_e \mathbf{p}_{\bar\nu} > 0$). An experiment done for the decay

$$\mathrm{Ne}^{19} \rightarrow \mathrm{F}^{19} + e + \bar\nu, \tag{24.68}$$

where the nuclear spin is 1/2 before and after the decay, showed that the latter is true, thus eliminating C_S.

Transitions which change the nuclear spin by one unit are sensitive to C_A^2 and C_T^2, with similar momentum correlations. The decay

$$\mathrm{He}^6 \rightarrow \mathrm{Li}^6 + e + \bar\nu \tag{24.69}$$

involves a change from nuclear spin 0 to 1. The electron and neutrino emerge antiparallel, so that $C_T^2 \approx 0$. Thus only C_V and C_A are appreciable.

The antineutrinos which appear in these decay have been found to interact very weakly with matter. Only many years later, in 1953, was it possible to detect them directly via the inverse reaction

$$\bar{\nu}_e + p \to n + e^+ \qquad (24.70)$$

using a strong antineutrino source of a large nuclear reactor filled with a high density of thermal neutrons.

After many precise measurements of angular correlations and electron and nuclear polarizations, the interaction was quite well determined to have the form

$$\mathcal{L} = -\frac{G}{\sqrt{2}}\bar{p}\gamma^\lambda\left(1-\frac{g_A}{g_V}\gamma_5\right)n[\bar{e}\gamma_\lambda(1-\gamma_5)\nu] + \text{c.c.}. \qquad (24.71)$$

with the coupling constant

$$G = (1.14730 \pm 0.000641) \times 10^{-5}\text{GeV}^{-2}, \qquad (24.72)$$

and the ratio

$$g_A/g_V = 1.255 \pm 0.006. \qquad (24.73)$$

The $\bar{e}\nu$ part of the interaction violates space reflection symmetry in the maximal possible way. Under parity, the left-helicity field $(1-\gamma_0)\nu(x)$ which possesses nonzero components only in the first two entries is multiplied by

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which moves the nonzero entries to the lower two components producing a right-helicity field $(1+\gamma_5)\gamma_0\nu$. This is not present in the Lagrangian. This maximal parity violation is responsible for the asymmetry of the decay electrons with respect to the neutron spin as observed in Madame Wu's experiment described on p. 182.

The ratio g_A/g_V can be measured in neutron decay via the up-down asymmetry in analogy with Madame Wu et al.'s experiment. The expectation $\langle \mathbf{s}_n \cdot \mathbf{p}_e \rangle$ is proportional to

$$|C_A|^2 + \text{Re}\, C_V C_A^* \propto (1 - g_A/g_V), \qquad (24.74)$$

The deviation of the ratio g_A/g_V from unity can be explained by strong interactions. That this is possible was first suggested by the weak decay of the 1937 discovered muon (intially mistaken with the pion). The muon decays weakly as follows

$$\mu^- \to e^- + \bar{\nu}_e + \nu_\mu. \qquad (24.75)$$

As was shown 1962 in an experiment in Brookhaven, the second antineutrino ν_μ which emerges in the decay has to be distinguished from that emerging in β-decay associated with the muon. The two neutrinos are referred to as muon antineutrino and electron antineutrino, respectively. With this assignment, the total number of electrons plus its electron neutrinos and the total number of muons plus muon neutrinos are both separately conserved (antiparticles are counted negatively). These laws are called *lepton number conservation laws*. The muon has no strong interaction and its decay is described by the interaction Lagrangian

$$\mathcal{L}_\mu = \frac{G_\mu}{\sqrt{2}}[\bar{\nu}_\mu \gamma^\lambda (1-\gamma_5)\mu][\bar{e}\gamma_\lambda(1-\gamma_5)\nu_e(x)] + \text{c.c.} + \ldots \ . \tag{24.76}$$

The value of G_μ is given by

$$G_\mu = (1.16632 \pm 0.00002) \times 10^{-5}\text{GeV}^{-2}. \tag{24.77}$$

It is larger than G_β by 2%.

The decay constant of the muon can be identified as the bare decay constant of weak interaction. In order to explain that the fact G_β is smaller than G_μ, Cabibbo, in 1964, put forward the hypothesis, that the reduction is due to the existence of a weak decay of strange particles. Studying the weak decays of

$$\begin{aligned} \Lambda &\rightarrow p + e^- + \bar{\nu}_e \\ \Sigma^+ &\rightarrow \Lambda + e^+ + \nu_e \end{aligned} \tag{24.78}$$

he observed that their weak coupling constant G^{strange} was considerably smaller than that of the neutrons. He noticed that he could explain the data quite well by assuming that

$$\begin{aligned} G &= \cos\theta_c G_\mu \\ G^{\text{strange}} &= \sin\theta_c G_\mu \end{aligned} \tag{24.79}$$

where

$$\theta_c = 0.21 \tag{24.80}$$

is the so-called *Cabibbo angle*.

Nowadays we believe that the weak interactions of all hadrons proceed via the decay of the quarks inside their wave functions. The non-strange hadrons decay by the elementary transition

$$\begin{aligned} d &\rightarrow u + e^- + \nu_e \\ d &\rightarrow u + \mu^- + \nu_\mu \\ u &\rightarrow d + e^+ + \bar{\nu}_c \\ u &\rightarrow d + \mu^+ + \bar{\nu}_\mu . \end{aligned} \tag{24.81}$$

The strange hadrons decay by the similar transition with the down quark d replaced by the strange quarks. Cabbibo's hypothesis amounts to the ansatz

$$\mathcal{L} = -\frac{G_\mu}{\sqrt{2}}\bar{u}\gamma^\lambda(1-\gamma_5)(\cos\theta_c\, d + \sin\theta_c\, s) \tag{24.82}$$

the quarks appear as combinations of the vector and axial vector currents

$$\begin{array}{cc} \bar{u}\gamma^{\lambda}d, & \bar{u}\gamma^{\lambda}\gamma_5 d, \\ \bar{u}\gamma^{\lambda}s, & \bar{u}\gamma^{\lambda}\gamma_5 s. \end{array} \tag{24.83}$$

It is important to realize that these are special components of the vector and axial vector currents which we found previously as conserved Nocther currents of QCD. In fact we can write

$$\begin{aligned} \bar{u}\gamma^{\lambda}d &= \sqrt{2}j^{\lambda}_{(1+i2)/\sqrt{2}} \equiv \sqrt{2}j_{\pi^+}, \\ \bar{u}\gamma^{\lambda}\gamma_5 d &= \sqrt{2}j_{5\,(1+i2)/\sqrt{2}} = \sqrt{2}j_{\pi^+}, \\ \bar{u}\gamma^{\lambda}s &= \sqrt{2}j_{(4+i5)/\sqrt{2}} = \sqrt{2}j_{K^+}, \\ \bar{u}\gamma^{\lambda}\gamma_5^{d} &= \sqrt{2}j_{5\,(4+i5)/\sqrt{2}} = \sqrt{2}j_{K^+}, \end{aligned} \tag{24.84}$$

where the subscripts π^+, K^+ indicate the SU(3) quantum numbers, the currents can create. The fact that the coupling constant of weak interactions carries the dimension mass out to be a great obstacle in calculating higher order correction to weak processes: The fact that the only successful field theory of fundamental interactions, quantumelectrodynamics, has only a three-particle interaction with the photon mediating the interactions, led to the hypothesis that weak interactions should be due to a similar coupling of a massive charged vector meson called W. As we shall see later in the analysis of perturbation theory, this would generate a weak coupling of the same type as in (24.71), but with G replaced by

$$G(q^2) = -\frac{e_W^2}{q^2 - M_W^2} \tag{24.85}$$

where q is the momentum carried off by the leptons and e_W the coupling strength of the heavy vector meson W to the leptons and nucleons. If M_W is much larger than 1 BeV, the q-dependence could be ignored and one would have

$$G_p \approx \frac{e_W^2}{M_W^2} \tag{24.86}$$

Since e_W is dimensionless it was suggestive to assume it to be equal to the coupling strength of the photons. Then weak interactions would carry only one more additional parameter, the mass of the vector meson. Using

$$e^2 = 4\pi\alpha \tag{24.87}$$

we find

$$M_W = \sqrt{\frac{4\pi\alpha}{G}} \approx 90\mathrm{GeV}. \tag{24.88}$$

A charged meson which has the desired properties and this was found near this predicted mass in 1983. Its precise mass is

$$M_W = 80\text{GeV}. \tag{24.89}$$

With the usual weak decays carring off a non-zero charge via the lepton, the question has been reaised whether weak interactions could also lead to a decay into $\nu_e\bar{\nu}_e, \nu_\mu\bar{\nu}_\mu, e\bar{e}$, or $\mu\bar{\mu}$. The first two could have easily escaped experimental detection, the last two would be hard to find since they would hide under the similar but much larger electromagnetic interaction. Such decays would come from couplings such as

$$\mathcal{L} = G^0\bar{u}\gamma^\mu(1-\gamma_5)u\{e\gamma_\mu e + \bar{\nu}_e(1-\gamma_5)\nu + (e \to \mu)\}. \tag{24.90}$$

The particle combinations $\bar{u}\gamma_\mu(1-\gamma_5)u$, $\bar{e}\gamma_\mu(1-\gamma_5)e$ do not change the charge of the decaying particles and are called *neutral currents*. Experimental evidence for such neutral currents has been found in 1973 in form of the purely leptonic reaction

$$\bar{\nu}_\mu + e^- \leftarrow \bar{\nu}_\mu + e^- \tag{24.91}$$

as well as in interactions

$$\begin{array}{ccc} \nu_\mu + \begin{matrix} u \\ d \end{matrix} & \longrightarrow & \nu_\mu + \begin{matrix} u \\ d \end{matrix} \\ \bar{\nu}_\mu + \begin{matrix} u \\ d \end{matrix} & \longrightarrow & \bar{\nu}_\mu + \begin{matrix} u \\ d \end{matrix}. \end{array} \tag{24.92}$$

Also a heavy neutral vector meson has been found which in analogy with W, mediates the neutral weak interactions. It is called Z boson and its mass is given by[5]

$$M_Z = 92.9 \pm 1.6\text{GeV}. \tag{24.93}$$

All these interactions plus the electromagnetic interactions wave unified in one field theory by Glashow, Weinberg, and Salam in the standard model of electromagnetic and weak electroweak interactions.

The free lepton Lagrangian for the electron part is

$$\mathcal{L} = (\bar{\nu}_{eL}, \bar{e}_{\rm L})\, \not{\partial} \begin{pmatrix} \nu_{eL} \\ e_{\rm L} \end{pmatrix} + \bar{e}_{\rm R} i \not{\partial}\, e_{\rm R} \tag{24.94}$$

It is invariant under an SU(2) group $\text{SU}_\text{L}(2)$ of the left-handed leptons and an SU(1) group $\text{U}_\text{R}(1)$ of the right-handed leptons where neutrino ν_R is absent. This Lagrangian is made locally $\text{SU}_\text{L}(2) \times \text{U}_\text{R}(1)$ invariant by means of two types of gauge fields. For the $\text{SU}_\text{L}(2)$ symmetry of the left-handed particles one uses a $2x2$ gauge field

$$W_\mu = W_\mu^a \frac{\tau_a}{2} \tag{24.95}$$

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[5] F.J. Habert et al, Phys. Lett. B *46*, 138 (1973); Nucl. Phys. B *73*, (1974).

where T_a acts on the two $\mathrm{SU_L}(2)$ isospin indices. Since these indices are mathematically equivalent to isospin, one speaks of a weak isospin. For the $\mathrm{SU_R}(1)$ symmetry of the right-handed electrons one uses a single vector field B_μ. The ordinary derivatives are replaced by the covariant derivatives

$$\begin{aligned} D_\mu &= \partial_\mu + igW_\mu \\ D_\mu &= \partial_\mu + ieB_\mu \end{aligned} \tag{24.96}$$

After this one introducies the dynamics to the gauge fields via the Lagrangian

$$\mathcal{L}_{\mathrm{GF}} = -\frac{1}{2}\mathrm{tr}\left[W_{\mu\nu}W^{\mu\nu}\right] - \frac{1}{4}F^2_{\mu\nu} \tag{24.97}$$

where

$$W_{\mu\nu} = \partial_\mu W_\nu - \partial_\nu W_\mu + ig[W_\mu W_\nu] \tag{24.98}$$

is the $\mathrm{SU}(2)_\mathrm{L}$ covariant curl and

$$F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu \tag{24.99}$$

the usual abelian curl.

Introducing the charged W meson fields

$$W^\pm_\mu = \frac{1}{\sqrt{2}}\left(W^1_\mu \pm iW^2_\mu\right), \tag{24.100}$$

the new interactions are

$$\begin{aligned} \mathcal{L}_{\mathrm{int}} &= -g(\bar{\nu}_{eL}\bar{e}_\mathrm{L})\gamma^\lambda W^a_\lambda \frac{T_a}{2}\begin{pmatrix} \nu_{eL} \\ e_\mathrm{L} \end{pmatrix} \\ &\quad -g'\bar{e}_\mathrm{R}\gamma^\lambda B_\lambda e_r \\ &= -g(\bar{\nu}_{eL}\bar{e}_\mathrm{L})\gamma^\lambda \begin{pmatrix} W^3_\lambda/2 & W^-_\lambda/\sqrt{2} \\ W^+_\lambda/\sqrt{2} & -W^3_\lambda/2 \end{pmatrix}\begin{pmatrix} \nu_{eL} \\ e_\mathrm{L} \end{pmatrix} \\ &\quad -g'\bar{e}_\mathrm{R}\gamma^\lambda B_\lambda e_\mathrm{R}. \end{aligned} \tag{24.101}$$

Actually, there is the same freedom in choosing the coupling constan g' associated with the vector meson B. We can always absorb an equal coupling to (ν_{ec}, e_L) into the term involving the field W^3. Hence we can write

$$-g'\bar{\nu}_{eL}\bar{e}_\mathrm{L}e_\mathrm{R}\gamma^\lambda Y \begin{pmatrix} \nu_{e_\mathrm{L}} \\ e_\mathrm{L} \\ e_\mathrm{R} \end{pmatrix} \tag{24.102}$$

where Y is called the *weak hypercharge* and has the form

$$Y = \begin{pmatrix} y_\mathrm{L} & & \\ & y_\mathrm{L} & \\ & & y_\mathrm{R} \end{pmatrix}. \tag{24.103}$$

The parameter $y_{\rm L}$ can be chosen at will since it can be absorbed into g, for instance

$$y_{\rm L} = 0. \tag{24.104}$$

Then the interaction reads

$$\begin{aligned}\mathcal{L}_{\rm int} &= -\frac{g}{\sqrt{2}}\left(W_\lambda^+ \bar{\nu}_{eL}\gamma^\lambda e_{\rm L} + \text{c.c.}\right)\\ &\quad -\frac{1}{2}\left(gW^3 - g'B_\lambda\right)\bar{\nu}_{eL}\gamma^\lambda \nu_{eL}\\ &\quad +\frac{1}{2}(qW_\lambda^3 + g'B_\lambda)\bar{e}_{\rm L}\gamma^\lambda e_{\rm L} + \frac{g'}{2}y_{\rm R}B_\lambda \bar{e}_{\rm R}\gamma^\lambda e_{\rm R}.\end{aligned} \tag{24.105}$$

Now we observe that the two fields W_λ^3 and B_λ being both massless allow for an arbitrary mixing. We introduce the physical photon field as

$$A_\mu = \cos\theta_W B_\mu + \sin\theta_W W_\mu^3 \tag{24.106}$$

and an orthogonal field which represents the neutral vector meson of weak interactions.

$$Z_\mu = -\sin\theta_W B_\mu + \cos\theta_W W_\mu^3. \tag{24.107}$$

The mixing angle is called *weak angle*. It is chosen so that the photon couples to the usual electromagnetic current which contains an equal amount of right-handed and left-handed electrons

$$j^\mu_{\rm em} = \gamma^\mu e_{\rm L} + \bar{e}_{\rm R}\gamma^\mu e_{\rm R}. \tag{24.108}$$

This fixes

$$\begin{gathered} y_{\rm R} = -1,\\ \sin\theta_W = \frac{g'}{\sqrt{g^2 + g'^2}}, \qquad \cos\theta_W = \frac{g}{\sqrt{g^2+g'^2}},\\ e = \frac{gg'}{\sqrt{g^2+g'^2}}, \end{gathered} \tag{24.109}$$

and the interaction becomes

$$\begin{aligned}\mathcal{L}_{\rm int} &= -\frac{g}{\sqrt{2}}\left(\bar{\nu}_{eL}\gamma^\lambda e_{\rm L}W_\lambda^+ + \text{c.c.}\right)\\ &\quad -\sqrt{g^2+g'^2}\left[\frac{1}{2}\left(\bar{\nu}_{eL}\gamma^\lambda\nu_{eL} - \bar{e}_{\rm L}\gamma^\lambda e_{\rm L}\right) + \sin^2\theta_W(e_{\rm L}\gamma^\lambda e_{\rm L} + \bar{e}_{\rm R}\gamma^\lambda e_{\rm R})\right] Z_\lambda\\ &\quad +gg'\frac{1}{2}(\bar{e}_{\rm L}\gamma^\lambda e_{\rm L} - \bar{e}_{\rm R}\gamma^\lambda e_{\rm R})A_\lambda.\end{aligned} \tag{24.110}$$

Expressed in terms of the electromagnetic current

$$j^\mu_{\rm em} = \bar{e}_{\rm L}\gamma^\mu e_{\rm L} + e_{\rm R}\gamma^\mu e_{\rm R} \tag{24.111}$$

we can write

$$\mathcal{L}_{\text{int}} = e\left[j^{\mu}_{\text{em}} A_{\mu} - -\frac{1}{\sin\theta_W}(j^{\mu}_{+} W^{+}_{\mu} + \text{c.c.}) + \frac{1}{\sin\theta_W} j^{\mu}_{\text{nc}} Z_{\lambda}\right]. \tag{24.112}$$

where

$$j^{\pm}_{\text{L}} = \frac{1}{\sqrt{2}}(\nu_{e_{\text{L}}} e_{\text{L}})\gamma^{\lambda}\tau^{\pm}\begin{pmatrix}\nu_{eL}\\ e_{\text{L}}\end{pmatrix} = \begin{Bmatrix}\bar{\nu}_{eL}\gamma^{\lambda}e_{\text{L}}\\ \bar{e}_{\text{L}}\gamma^{\lambda}\nu_{eL}\end{Bmatrix} \tag{24.113}$$

$$j^{3}_{\text{L}} = (\nu_{e_{\text{L}}}, \bar{e}_{\text{L}})\gamma^{\lambda}\frac{\tau^{3}}{2}\begin{pmatrix}\nu_{e_{\text{L}}}\\ e_{\text{L}}\end{pmatrix} = \frac{1}{2}(\nu_{eL}\gamma^{\lambda}\nu_{eL} - \bar{e}_{\text{L}}\gamma^{\lambda}e_{\text{L}}) \tag{24.114}$$

are the left-handed weak currents written as vectors in the *weak isospace* and

$$j_{\text{nc}} = j^{3}_{\text{L}} + \sin^2\tau_W j_{\text{em}} \tag{24.115}$$

is the *neutral current*. The weak angle describes the admixture of the ordinary electric current to the neutral weak isospin current.

Up to this point, the model had been constructed at the phenomenological level by Glashow in 1961. He added to the Lagrangian mass terms for the W and the Z meson

$$\frac{M_W^2}{2}\left(W^{+2} + W^{-2}\right) + \frac{M_Z^2}{2} Z^2 \tag{24.116}$$

choosing the value for M_W which gives the correct weak coupling constant not knowing what to choose for M_Z. In this way he obtained a model which parametrized the known weak interactions and predicted the unknown neutral currents.

The weak interaction with quarks are incorporated by adding the Lagrangian

$$\begin{aligned}\mathcal{L}_{\text{int}} &= \frac{g}{2\sqrt{2}}\left(W^{+}_{\mu} j^{+}_{h} + \text{c.c.}\right) + eA^{\mu} j^{\text{em}}_{\mu}\\ &\quad -\sqrt{g^2 + g'^2} Z^{\mu}\left(\bar{q}_{\text{L}}\frac{\tau_3}{2}\gamma_{\mu}q_{\text{L}} - \sin^2\theta_W j_{h\,\text{em}})\theta_{\omega}{}^{j}\right)\mu_h{}^{\text{em}}\end{aligned} \tag{24.117}$$

where

$$\begin{aligned}j^{+}_{h} &= \bar{u}_{\text{L}}\gamma_{\mu}(d_{\text{L}}\cos\theta_c + s_{\text{L}}{}^{i}\theta_c)\\ h_{h\,\text{em}} &= \frac{2}{3}\bar{u}\gamma_{\mu}u - \frac{1}{3}\left(\bar{d}\gamma_{\mu}d + \bar{s}\gamma_{\mu}s\right)\end{aligned} \tag{24.118}$$

When the theory got to this stage it was realized that it contained an unpleasant contradiction with experiments. The neutral vector meson Z was coupled to a quark current

$$\begin{aligned}\bar{q}_{\text{L}}\gamma^{\mu}\tau_3 q_{\text{L}} &= \bar{u}_{\text{L}}\gamma_{\mu}u_{\text{L}} - \cos^2\theta_c\bar{d}_{\text{L}}\gamma_{\mu}d_{\text{L}}\\ &\quad -i\sin\theta_c\cos\theta_c\left(\bar{d}_{\text{L}}\gamma_{\mu}s_{\text{L}} + \bar{s}_{\text{L}}\gamma_{\mu}d_c\right) - i\sin^2\theta_c\bar{q}_{\text{L}}\gamma_{\mu}c_{\text{L}}.\end{aligned} \tag{24.119}$$

The third term changes the strangeness by one unit. Processes with a strangeness-changing neutral current are, however, strongly suppressed in nature. Otherwise the particle decays

$$\begin{aligned} K^{\pm} &\rightarrow \pi^{\pm}\nu\bar{\nu} \\ K^0 &\rightarrow \mu^+\mu^- \end{aligned} \tag{24.120}$$

would have a much larger branching ratio than the experimentally observed $6 \times 10^{-7}, 10^{-8}$, respectively (see Fig. 24.1). In order to achieve the desired suppression,

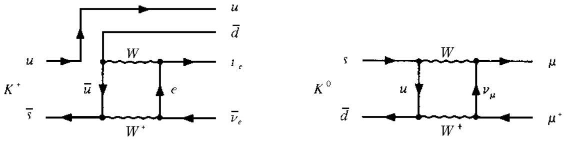

FIGURE 24.1 Quark diagrams for K^+ and K^0 decays involving strangeness changing neutral currents.

Glashow, Iliopolous, and Maiani[6] postulated the existence of a further quark, called charmed quark and denoted by c, which was suppressed to form a weak isodoublet with s in the same way as u does with d. They then considered the two doublets

$$\begin{pmatrix} u \\ d_\theta \end{pmatrix}_{\rm L}, \begin{pmatrix} c \\ s_\theta \end{pmatrix}_{\rm L} \tag{24.121}$$

as two families of the same sort, both with weak hypercharge 1/3, and wrote the left-handed neutral current as

$$\left(\bar{u}, \bar{d}_\theta\right) \frac{\tau_3}{2}\gamma^\mu \begin{pmatrix} u \\ d_\theta \end{pmatrix}_{\rm L} + \left(\bar{c}, \bar{s}_\theta\right) \frac{\tau_2}{2}\gamma^\mu \begin{pmatrix} c \\ s_\theta \end{pmatrix}_2 - i\sin^2\theta_W j^\mu_{\rm em} \tag{24.122}$$

Now the strangeness changing currents cancel exactly. The cancellation in the above K decays goes as follows. Take, for instance, $K \rightarrow \mu^+\mu^-$, where the compensating diagrams are shown in Fig. 24.2.

To the electromagnetic current, the charmed quark contributes an additional

$$\frac{2}{3}\bar{c}\gamma_\mu c.$$

Unfortunately, the model as it stood still had an important handicap which prevented it from becoming a bona fide quantum field theory of electronical interactions.

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[6] S.L. Glashow, J. Iliopolous, L. Maiani, Phys. Rev. D *2*, 1285 (1970).

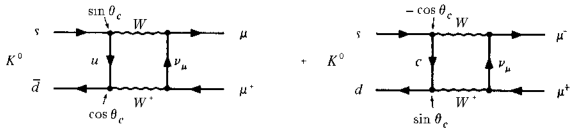


FIGURE 24.2 Diagrams for the $K^0 \to \mu^+\mu^-$ decay with compenstaing strangeness-changing neutral currents.

Just as the four-fermi theory, it does allow for higher order perturbation correction. The infinites appearing in higher order cannot be renormalized away. The reason is the presence of the explicit mass terms. We shall see later that further symmetry is necessary to allow for a renormalization. The action must be assumed to be invariant under the local $\mathrm{SU(2)_L \times U(1)_R}$ gauge group which was used to construct the interactions. It is this gauge group which permits the renormalization of the theory. The initial Lagrangian contains only massless $W^{\pm}$ and Z mesons To have massive W and Z mesons it is necessary to generate these masses spontaneously, by an effect which was known from superconductivity as the *Meissner effect*. The vector potential of magnetism in a superconductor becomes massive when entering the superconductive phase. These aspects will be discussed later.

Notes and References

In Monte Carlo simulations of lattice gauge theories, the mass spectrum of hyperons with b-quarks has been calculated by
C. Alexandrou, A. Borelli, S. Güsken, F. Jegerlehner, K. Schilling, G. Siegert, R. Sommer, et al., hep-lat/9407027

25

Critical Properties of Non-linear σ-Model

25.1 INTRODUCTORY REMARKS

The $4-\epsilon$ -expansion of O(N)-symmetric φ^4-theories is not the only technique to study critical phenomenon of three-dimensional systems with O(N)-symmetry. A great deal can be learned about such systems by ignoring the size fluctuations of the fields and focusing attention only upon the Goldstone modes of the system, which are present in the ordered phase. We have explained before in Chapter 9 that in the limit of very low temperature or strongly negative mass parameter m^2, the fields φ_a, $a = 1\dots\ N$ in a $\left(\varphi_a^2\right)^2$-theory

$$\mathcal{A} = \int d^dx \left[\frac{1}{2}\left(\partial\varphi_a\right)^2 + \frac{m^2}{2}\varphi_a^2 + \frac{g}{4}\left(\varphi_a^2\right)^2\right] \tag{25.1}$$

acquire an infinite mass

$$M^2 = -2m^2 \to \infty \tag{25.2}$$

and are practically frozen at a fixed size

$$\varphi_a^2 = |\varphi|^2. \tag{25.3}$$

Only the italic of φ_a are fluctuating easily. If these directions are denoted by the unit vectors $n_a = \varphi_a/\varphi$, the action describing these fluctuations can be written as

$$\mathcal{A} = \frac{1}{2t}\int d^Dx\left(\partial n_a\right)^2, \qquad n_a^2 = 1 \tag{25.4}$$

where $1/t = |\varphi|^2$. The partition function is defined by functionally integrating $e^{-\mathcal{A}}$ over all directions at each space point. The measure of integration is

$$\begin{aligned}\int \mathcal{D}\mathbf{n} &= \prod_{x,a}\int_{-\infty}^{\infty}\frac{d^Nn_a(x)}{S_N}\delta^{(D)}\left(n_a^2-1\right)\\ &= \prod_{x,a}\int\frac{d^{N-1}n_a(x)}{S_N},\end{aligned} \tag{25.5}$$

where S_N is the surface of the sphere in the N-dimensional space, i.e., $S_N = 2\pi^{N/2}/\Gamma(N/2)$. The partition function is therefore

$$Z = \int \left[\frac{\mathcal{D}\mathbf{n}}{S_N}\right] e^{-\mathcal{A}[\mathbf{n}]}. \tag{25.6}$$

As mentioned above, this is the continuum version of the so-called classical O(N)-Heisenberg model of magnetism on a lattice

$$Z = \prod_{\mathbf{x},a}\left[\int \frac{d\mathbf{n}(\mathbf{x})}{S_N}\right] \exp\left\{\frac{1}{2T}\sum_{\mathbf{x},i}\left[(\nabla_i n_a(\mathbf{x}+\mathbf{i}))^2 + 2D\right]\right\} \tag{25.7}$$

where $\nabla_i n(\mathbf{x}) = n(\mathbf{x}) + \mathbf{i} - n(\mathbf{x})$ are the differences of $n^a(\mathbf{x})$ between sites. Because of this connection, we shall rename g as t and speak about it as a temperature. In Chapter 9 we have solved this model exactly in the limit $N \to \infty$, and the reader is referred to this chapter to recapitulate some of the results.

We shall now calculate the partition function (25.6) perturbativey for arbitrary N. For this we select a particular orientation of the direction vector n_a, say $N_a = (0,0,0,0,1)$, as a reference direction state, and consider the first $N-1$ components

$$\pi_a(x) \equiv n_a(x); \qquad a = 1,\dots,N-1 \tag{25.8}$$

as independent fields of the system. The Nth component is then determined from the others by the unit length:

$$n_N(x) = \sqrt{1-\pi_a^2(x)} \equiv \sigma(x), \tag{25.9}$$

and we can write the action of the non-linear σ model as

$$\mathcal{A} = \frac{1}{2t}\int d^Dx \left[(\partial\pi_a)^2 + \left(\partial\sqrt{1-\pi_a^2}\right)^2\right] \tag{25.10}$$

This action is scale invariant for $D = 2$ dimensions in, where the field π_a has a vanishing naive dimension. The theory is renormalizable by power counting. Below $D = 2$ dimensions, the fluctuations are so violent that massless excitations do not exist. All Goldstone modes become massive at all temperature. The dimension $D = 2$ is called the *lower critical dimension.*

For the action (25.4), the measure of integration is found by performing in (25.5) the integral over $n_N(x)$ after which remain with

$$\int \frac{\mathcal{D}^{N-1}\boldsymbol{\pi}}{\sqrt{1-\boldsymbol{\pi}^2}} = \prod_{x,a=1}^{N-1}\int \frac{d\pi_a(x)}{\sqrt{1-\pi_a^2(x)}}. \tag{25.11}$$

This can also be written as

$$\prod_{x,a=1}^{N-1}\int \mathcal{D}^{N-1}\pi_a \exp\left\{-\frac{1}{2a^D}\int d^Dx \log\left(1-\pi_a^2(x)\right)\right\}, \tag{25.12}$$

where we have assumed the path integral to be set up on an underlying simple lattice of spacing a, such that we may write the products over all space points as exponentials of sums, which are turned into integrals:

$$\prod_x f(x) = \exp\left[\sum_x \log f(x)\right] = \exp\left[\frac{1}{aD}\int d^D x \log f(x)\right]. \tag{25.13}$$

Then the partition function (25.6) of the non-linear σ model becomes

$$\begin{aligned} Z \;=\; \prod_{x,a=1}^{N-1}\left[\int \mathcal{D}^{N-1}\pi_a\right] \exp\Bigg\{-\frac{1}{2t}\int d^D x\left[(\partial\pi_a)^2 + \left(\partial\sqrt{1-\pi_a^2}\right)^2\right] \\ -\frac{1}{2a^D}\int d^D x \sum_{a=1}^{N-1}\log\left[1-\pi_a^2(x)\right]\Bigg\}. \end{aligned} \tag{25.14}$$

Note that the original O(N)-invariance of the Lagrangian (25.228) under transformation

$$\delta n_a = \omega_{ab}\,\delta n_b, \tag{25.15}$$

with $\omega_{ab} = -\omega_{ba}$, is present in (25.4) for transformations

$$\begin{aligned} \delta\pi_a &= \omega_{ab}\,\delta\pi_b + \omega_{aN}\sqrt{1-\pi_c^2}, \\ \delta\sqrt{1-\pi_c^2} &= -\omega_{aN}\,\delta\pi_a. \end{aligned} \tag{25.16}$$

25.2 PERTURBATION THEORY

For a perturbation calculation of (25.14) we identify the free action as

$$\mathcal{A}_0 = \frac{1}{2t}\int d^D x (\partial\pi_a)^2, \tag{25.17}$$

and consider the remaining terms as interactions:

$$\begin{aligned} \mathcal{A}_{\text{int}} \;=\; \int d^D x\Bigg\{\frac{1}{2t}\left[\frac{1}{4}\left(\partial\pi_a^2\right)\left(\partial\pi_b^2\right) - \frac{3}{16}\left(\partial\pi_a^2\right)\partial\left(\pi_b^2\right)^2 + \dots\right] \\ -\frac{1}{2a^D}\pi_a^2(x) - \frac{1}{4a^D}\left(\pi_a^2\right)^2\frac{1}{6a^D}\left(\pi_a^2\right)^3 - \dots\Bigg\} \end{aligned} \tag{25.18}$$

The functional integration is limited to the regime $\boldsymbol{\pi}^2 < 1$, to be covered twice, once for $\sigma = +\sqrt{1-\boldsymbol{\pi}^2}$ and once for $\sigma = -\sqrt{1-\boldsymbol{\pi}a^2}$. The perturbation expansion is a power series in t. For small t, the fluctuations will take place in the neighborhood of $\boldsymbol{\pi}^2 \sim 0$. One may therefore replace the integrations over each field component $\pi_a(x)$ by ba one from $-\infty$ to ∞, committing an error of the order $e^{-1/t}$. With this replacement, the free propagator is

$$\begin{aligned} \langle\pi_a(x)\pi_b(y)\rangle &= \delta_{ab}\int\frac{d^D k}{(2\pi)^D}\frac{t}{k^2}e^{ik(x-y)} \\ &\equiv \delta_{ab}G_0(x-y). \end{aligned} \tag{25.19}$$

Observe that the $\boldsymbol{\pi}^2$-term coming from the measure is not considered as being part of the free-field action, but is treated as an interaction term since it carries a factor t.

In order to avoid problems with singularities at $k = 0$ (infrared singularities), it is useful to place the system into an external field pointing along the preferred $a = N$ direction:

$$\mathcal{A}_{\rm ext} = -\frac{h}{t}\int d^Dx\,\sigma = -\frac{h}{t}\int d^Dx\sqrt{1-\pi_a^2}. \tag{25.20}$$

This corresponds to putting the Heisenberg model of magnetism into an external magnetic field. This field serves to stabilize the selected preferred direction along $n^a = (0, 0, 0, \dots, 1)$ which was chosen to define the fields π_a. Expanding also $\mathcal{A}_{\rm ext}$ in powers of π_a, this replacement produces a pion mass term in the action

$$\mathcal{A}_m = \frac{h}{2}\int d^Dx\,\pi_a^2(x), \tag{25.21}$$

which changes the free propagator into

$$G_0(x-y) = \int \frac{d^Dk}{(2\pi)^D}e^{ik(x-y)}\frac{t}{k^2+m^2} \tag{25.22}$$

where

$$m^2 = h. \tag{25.23}$$

It also adds a further set of interactions

$$\mathcal{A}_{\rm int} = m^2\int d^Dx\left[-1+\frac{1}{8}\left(\pi_b^2\right)^2+\frac{1}{16}\left(\pi_b^2\right)^3+\dots\right], \tag{25.24}$$

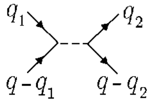
the first being a trivial shift in the energy. In momentum space, the lowest interactions in (25.18) can be written as follows

2-point

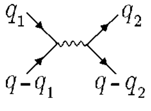
$$= -\frac{1}{4a^D}\int \mathrm{d}^Dq\;\pi_a(q)\pi_a(-q), \tag{25.25}$$

$$\tag{25.26}$$

4-point

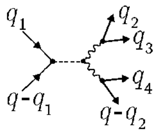


$$= \frac{1}{8t}\int \bar{d}^Dq_1\int \mathrm{d}^Dq_2\int d^Dq(q^2+m^2)\pi_a(q_1)\pi_a(q-q_1)\pi_b(-q_2)\pi_b(q_2-q), \tag{25.27}$$

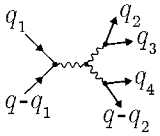


$$= -\frac{1}{4a^D}\int \bar{d}^Dq_1\int \bar{d}^Dq_2\int \bar{d}^Dq\;\pi_a(q_1)\pi_a(q-q_1)\pi_b(-q_2)\pi_b(q_2-q), \tag{25.28}$$

6-point



$$= -\frac{1}{16t}\int \bar{d}^D q_4 \cdots \int \bar{d}^D q \left(q^2+m^2\right) \times \tag{25.29}$$
$$\times \pi_a(q_1)\,\pi_a(q-q_1)\,\pi_b(-q_2)\,\pi_b(-q_3)\,\pi_c(-q_4)\,\pi_c(q_2+q_3+q_4-q)\,,$$



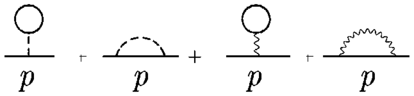
$$= -\frac{1}{6a^D}\int \bar{d}^D q_1 \cdots \int \bar{d}^D q_4 \int \bar{d}^D q \tag{25.30}$$
$$\times \pi_a(q_1)\pi_a(q-q_1)\,\pi_b(-q_2)\,\pi_b(-q_3)\,\pi_c(-q_4)\,\pi_c(q_2+q_3+q_4-q)\,.$$

The dashed line stands for a factor q^2+m^2, while the wiggly lines represent a local interaction. In addition, these lines indicate the contraction of the O(N)-exponents of the pairs of π-lines emerging from its ends.

From the magnetic interaction (25.20) we obtain once more the lower two-point interaction with a prefactor $m^2/8t$, and the lower four-point interaction with a prefactor $m^2/16t$, etc.

We shall now study the renormalization of the propagator to lowest order in perturbation theory. The self-energy contains two contractions involving the four-point function:

$\Sigma(p) =$



. (25.31)

Let us calculate the first two diagrams using (25.27) and closing two lines by a propagator. Alternatively, we may calculate the expectation

$$\frac{1}{8t}\int \bar{d}^D q_1 \int \bar{d}^D q_2 \int \bar{d}^D q\;(q^2+m^2)\langle \pi_c(p)\pi_a(q_1)\,\pi_a(q-q_1)\,\pi_b(-q_2)\,\pi_b(q_2-q)\,\pi_d(-p)\rangle$$

form all Wick contractions, remove the disconnected diagrams, and amputate the external legs. This gives

$$\begin{aligned}
2\int \bar{d}^D q_1 \int \bar{d}^D q_2 \int \bar{d}^D q\,(q^2+m^2)\Bigg\{&(N-1)\delta_{ca}\,\delta^{(D)}(p+q_1)\,\delta_{ad}\,\delta^{(D)}(q-q_1-p)\,\frac{\delta^{(D)}(-q)}{q_2^2+m^2}\\
&+2\delta_{ca}\,\delta^{(D)}(p+q_1)\,\delta_{ab}\frac{\delta^{(D)}(q-q_1-q_2)}{(q-q_1)^2+m^2}\delta^{(D)}(q_2-q-p)\Bigg\}\\
=\delta_{cd}\,\frac{1}{2}\int \bar{d}q^D &\left\{(N-1)\frac{m^2}{q^2+m^2}+2\frac{q^2+m^2}{(p+q)^2+m^2}\right\}.
\end{aligned} \tag{25.32}$$

By rewriting

$$\int \bar{d}^D q\frac{q^2+m^2}{(q+p)^2+m^2} = \int \bar{d}^D q\frac{(q+p)^2+m^2-2p(q+p)+p^2}{(q+p)^2+m^2}, \tag{25.33}$$

we can drop the $p(q+p)$-term, since it is odd in $(q+p)$, and (25.33) becomes

$$= \int \bar{d}^D q + p^2 \int \bar{d}^D q \frac{1}{q^2+m^2}. \tag{25.34}$$

On a lattice, the first integral is equal to

$$\frac{1}{Na^D} \sum_q = \frac{1}{aD}, \tag{25.35}$$

where N is the number of cells in the underlying lattice. Hence we can identify

$$\int \bar{d}^D q = \frac{1}{a^D}. \tag{25.36}$$

This term in (25.34) is precisely cancelled by the contribution of the two-point interaction (25.26), and we arrive at

$$\sigma_{cd}(p) = \delta_{cd} \left[\frac{1}{2} (N-1)\, m^2 + p^2 \right] L \tag{25.37}$$

where L is the one-loop integral

$$L \equiv \int \bar{d}^D q \frac{1}{q^2+m^2}. \tag{25.38}$$

The two-point vertex function is therefore at the one-loop level

$$\Gamma^{(2)}_{cd}(p) = \delta_{cd} \left\{ \frac{1}{t} \left(p^2 + m^2 \right) + \left[\frac{1}{2}(N-1)m^2 + p^2 \right] L \right\}. \tag{25.39}$$

A one-loop effective action would have a free-field part

$$\mathcal{A}_{\text{eff}}[\pi] = \int d^d x \; \pi_c(x) \Gamma^{(2)}_{cd}(-i\partial) \pi_d(x) \tag{25.40}$$

The resulting two-point vertex function is thus

$$\Gamma^{(2)}_{cd}(p) = \delta_{cd} \left\{ \frac{1}{t} \left(p^2 + m^2 \right) + \left[\frac{1}{2}(N-1)m^2 + p^2 \right] L \right\} + \mathcal{O}(t). \tag{25.41}$$

The corresponding effective action has a free-field part

$$\mathcal{A}_{\text{eff}}[\pi] = \int d^D x \; \Pi_c(x) \Gamma^{(2)}_{cd}(-i\partial) \Pi_d(x), \tag{25.42}$$

and reads in x-space

$$\mathcal{A}_{\text{eff}} = \frac{1}{2} \int d^D x \left\{ \left[\frac{1}{t} + L \right] (\partial \Pi_a)^2 - \frac{h}{t} \left[1 + \frac{1}{2} (N-1)\, tL \right] \Pi_a^2 \right\}. \tag{25.43}$$

These are the same field expressions as in the original free-field action, except that t and h^2 are replaced by the renormalized values,

$$\begin{aligned} \frac{1}{t} &\rightarrow \frac{1}{t} + L \\ h &\rightarrow h\left[1 + \frac{1}{2}(N-1)tL\right]. \end{aligned} \tag{25.44}$$

The surprising feature of this theory is that due to the O(N)-symmetry, the renormlized action to all orders can be described in terms of only two renormalization constants, a wave function renormalization

$$\pi_R = Z_\pi^{-1/2}\pi \tag{25.45}$$

and a temperature renormalization

$$t_R = Z_t^{-1}t. \tag{25.46}$$

The symmetry forces us to introduce the renormalized magnetic field h as

$$h_R = Z_t^{-1}Z_\pi^{1/2}h \equiv Z_h h. \tag{25.47}$$

This will be soon be demonstrated to any order on general grounds. Supposing, for a moment, that this is true we write the renormalized free part of the effective action as

$$\mathcal{A}_{\rm eff} = \frac{1}{2t_R}\int d^Dx\left[(\partial\pi_R)^2 + h_R\pi_R^2\right]. \tag{25.48}$$

Comparison with (25.44) gives

$$\begin{aligned} Z_t Z_\pi^{-1} &= (1 - tL) \\ Z_\pi^{-1/2} &= \left(1 + \frac{N-1}{2}tL\right) \end{aligned} \tag{25.49}$$

and hence

$$\begin{aligned} Z_\pi &= 1 - (N-1)\,tL + \dots, \\ Z_t &= 1 - (N-2)\,tL + \dots, \end{aligned} \tag{25.50}$$

$$Z_h = Z_t^{-1}Z_\pi^{1/2} = 1 + \frac{N-3}{2}tL + \dots\,. \tag{25.51}$$

Thus the temperature is renormalized as follows

$$\frac{1}{t_R} = \frac{1}{t} - (N-2)\,L + \dots\,. \tag{25.52}$$

For the simplest case of an O(2)-model, this implies *no* first-order renormalization of the temperature at all, i.e., the coupling strength of the π_a-fields is unchanged by fluctuations. This property turns out to hold at *all* orders in t.

Obviously, this result depends crucially on the way the two renormalization factors in (25.43) are distributed over wave function and temperature. It is therefore worthwhile to go through the general renormalization in some detail.

It is interesting to point out a property of this field theory in $D = 1$ dimensions where we may interpret x as an imaginary time τ and $\pi_a(x)$ as a position variable $x_a(\tau)/R$ of a point particle on the surface of a sphere of radius $R = 1/\sqrt{t}$ in N dimensions. The comparison will be presented in Section 25.8

25.3 SYMMETRY PROPERTIES OF RENORMALIZED EFFECTIVE ACTION

The O(N)-symmetry of the theory implies the existence of a Ward-Takahashi identity which has to be fulfilled by the generating functional of all correlation functions:

$$Z[j_a,h] = \int \frac{\mathcal{D}\boldsymbol{\pi}}{\sqrt{1-\boldsymbol{\pi}^2}} \exp\left\{-\frac{1}{t}\int d^Dx\,(\partial\pi_a)^2 + \left(\partial\sqrt{1-\pi_a^2}\right)^2 - j_a\pi_a - h\sqrt{1-\pi_a^2}\right\}. \tag{25.53}$$

Under a rotation in each of the (N,a)-planes for $a = 1,\dots,N-1$, by an angle $\omega_{aN} \equiv \omega_a$:

$$\begin{aligned} \delta\pi_a &= \omega_a\sqrt{1-\pi_c^2}, && (25.54)\\ \delta\sqrt{1-\pi_a^2} &= -\omega_a\pi_a, && (25.55) \end{aligned}$$

the source terms go over into

$$\begin{aligned} &\int d^Dx\left\{j_a\pi_a h\sqrt{1-\pi_a^2} + \left[j_a\sqrt{1-\pi_c^2} - h\pi_a\right]\omega_a\right\}\\ &\qquad = \int d^Dx\left[(j_a - h\omega_a)\,\pi_a + (h + j_a\omega_a)\sqrt{1-\pi_c^2}\right]. \end{aligned} \tag{25.56}$$

This implies that $Z[j_a,h]$ must be invariant under the replacement

$$\begin{aligned} j_a &\rightarrow j_a + h\omega_a, && (25.57)\\ h &\rightarrow h - j_a\omega_a, && (25.58) \end{aligned}$$

which changes $Z[j_a,h]$ by

$$\delta Z[j_a,h] = \left[\left(h\frac{\partial}{\partial j_a} - \partial_a\frac{\partial}{\partial h}\right)Z\right]\omega_a. \tag{25.59}$$

This change has to vanish for any ω_a.

In order to find the consequences for the connected correlation functions, we go over to their generating functional

$$W[j_a, h] = -t \log Z[j_a, h]. \tag{25.60}$$

Defining the effective fields as usual by the functional derivatives of $W[j_a, h]$ with respect to the currents,

$$\Pi_a \equiv -\frac{\partial W}{\partial j_a}, \tag{25.61}$$

the effective energy at a fixed magnetic field h is given by the Legendre transform

$$\Gamma\,[\Pi_a, h] = W[j_a, h] + \int d^D x\ \Pi_a(x) j_a(x), \tag{25.62}$$

which contains the information on the currents in the derivative

$$j_a = \frac{\partial \Gamma}{\partial \Pi_a}. \tag{25.63}$$

The symmetry property (25.59) of $Z[j_a, h]$ can then be expressed as

$$\int d^D x \left[h(x)\Pi_a(x) + \frac{\delta \Gamma}{\delta h(x)} \frac{\delta \Gamma}{\delta \Pi_a(x)} \right] = 0 \tag{25.64}$$

We now separate $\Gamma[\Pi_a, h]$ into an h-free part $\Gamma^{(0)}[\Pi_a]$, and a part containing h. Since h is small, we may keep only the linear term in h, and continue with

$$\Gamma[\Pi_a, h] = \Gamma^{(0)}[\Pi_a] + \int d^D x\ h(x)\Gamma^{(1)}[\Pi_a](x) + \dots\ . \tag{25.65}$$

For the first two expansion terms, Eq. (25.64) implies

$$\begin{aligned} \int d^D x\ \Gamma^{(1)}[\Pi_a](x) \frac{\delta \Gamma^{(0)}[\Pi_a]}{\delta \Pi_a(x)} &= 0 && (25.66)\\ \int d^D x' \left\{ \Pi_a(x') + \Gamma^{(1)}[\Pi_a](x') \frac{\delta \Gamma^{(1)}[\Pi_a](x)}{\delta \Pi_a(x')} \right\} &= 0. && (25.67) \end{aligned}$$

For the further discussion we shall consider only the case of two dimensions, where the action is scale invariant and renormalizable by power counting. We focus attention upon the divergent part of the effective action, which also satisfies the differential equations (25.66), (25.67). Since the theory is renormalizable, the infinities appear only in quite restricted functional forms, the terms which have the same form as those in the original, i.e., $\int d^2x(\partial\Pi_a)^2$ and $\int d^2x(\Pi_a^2)^n$. Thus we only need to search for solutions of (25.66) among (25.67) quite restricted local functionals. In fact, the search for the expansion coefficient $\Gamma^{(1)}[\Pi_a](x)$ can be restricted even more.

Since h has dimension two, $\Gamma^{(1)}[\Pi_a](x)$ must be dimensionless. This implies that in a functional expansion of $\Gamma^{(1)}[\Pi_a](x)$,

$$\begin{aligned}\Gamma^{(1)}[\Pi_a](x) &= \Gamma^{(1)}[0](x) + \int d^2y\, \Gamma^{(1)\prime}[0](x,y)\delta\Pi_a(y) \\ &\quad + \frac{1}{2}\int d^2y d^2z\, \Gamma^{(1)\prime\prime}[0](x,y)\delta\Pi_a(y)\delta\Pi_a(z) + \dots, \end{aligned} \tag{25.68}$$

the only coefficients permitted on dimensional grounds are $\delta^{(2)}$-functions, i.e., $\Gamma^{(1)}[\Pi_a](x)$ is not only a local functional but even a *function* of $\Pi_a(x)$:

$$\Gamma^{(1)}[\Pi_a](x) = \gamma^{(1)}\left(\Pi_a(x)\right). \tag{25.69}$$

Thus Eq. (25.63) implies

$$\frac{\partial\gamma^{(1)}}{\partial\Pi_a}\gamma^{(1)} + \Pi_a = 0 \tag{25.70}$$

which can be integrated right-away to give

$$\gamma^{(1)}\left(\Pi_a(x)\right) = \sqrt{B - \Pi_a^2(x)}. \tag{25.71}$$

The h-free term $\Gamma^{(0)}[\Pi_a]$ must reflect the O(N)-invariance. Hence it must have the form

$$\Gamma^{(0)}[\Pi_a] = \int d^Dx A\left\{\frac{1}{2}\left(\partial\Pi_a\right)^2 + \frac{1}{2}\left(\partial\sqrt{C-\Pi_a^2}\right)^2\right\} \tag{25.72}$$

with some arbitrary constant A and C.

The point is now that due to the identity (25.66), the constants C and B are not independent. Indeed, since

$$\begin{aligned}\frac{\delta\Gamma^{(0)}}{\delta\Pi_a} &= -\partial^2\Pi_a + \frac{\delta}{\delta\Pi_a}\frac{1}{2}\int d^2x\frac{(\Pi_c\partial_i\Pi_c)^2}{C-\Pi_d^2} \\ &= -\partial^2\Pi_a + \frac{\partial_i\Pi_a\partial_i\Pi_c}{C-\Pi_d^2} + \frac{\Pi_a}{(C-\Pi_d^2)}(\Pi_c\partial_i\Pi_c)^2 - \partial_i\left[\frac{\Pi_a}{\sqrt{C-\Pi_d^2}}\frac{\Pi_c\partial_i\Pi_c}{\sqrt{C-\Pi_d^2}}\right] \\ &= -\partial^2\Pi_a + \frac{\Pi_a}{\sqrt{C-\Pi_d^2}}\partial_i^2\sqrt{C-\pi_d^2}, \end{aligned} \tag{25.73}$$

we can write (25.66) as

$$\int d^2x\sqrt{B-\Pi_a^2}\left[-\partial^2\Pi_a + \frac{\Pi_a}{\sqrt{C-\pi^2}}\partial^2\sqrt{C-\Pi_d^2}\right] = 0. \tag{25.74}$$

Partial integrations on the first term brings this to

$$\int d^2x\left[-\Pi_a\partial^2\sqrt{B-\Pi_c^2} + \sqrt{\frac{B-\Pi_c^2}{C-\Pi_d^2}}\partial^2\sqrt{C-\Pi_c^2}\right] = 0, \tag{25.75}$$

and we conclude that the two constants B and C must be identical. The terms in the effective action with divergences have therefore the general form

$$\Gamma^{(0)}[\Pi_a] = \frac{1}{t}\int d^2x \left\{\frac{A}{2}(\partial_i\Pi_a)^2 + \frac{A}{2}\left(\partial_i\sqrt{B-\Pi_a^2}\right)^2 - h\sqrt{B-\Pi_a^2}\right\}. \tag{25.76}$$

This can be brought to the original form by introducing renormalized quantities

$$\Gamma^{(0)}[\Pi_a] = \frac{1}{t_R}\int d^2x \left\{\frac{1}{2}(\partial_i\Pi_{Ra})^2 + \frac{1}{2}\left(\partial_i\sqrt{1-\Pi_{Ra}^2}\right)^2 - h_R\sqrt{1-\Pi_{Ra}^2}\right\} \tag{25.77}$$

If we rewrite (25.76) as

$$\begin{aligned}\Gamma^{(2)}[\Pi_a] \;=\; & \frac{AB}{t}\int d^2x \left\{\frac{1}{2}\left[\partial(B^{1/2}\Pi_a)\right]^2\right.\\ & \left.+\frac{1}{2}\left[\partial\sqrt{1-(B^{-1/2}\Pi_a)^2}\right]^2 - hA^{-1}B^{-1/2}\sqrt{1-(B^{-1/2}\Pi_a)^2}\right\},\end{aligned} \tag{25.78}$$

we identify

$$\begin{align}\Pi_{Ra} &= B^{-1/2}\Pi_a, \nonumber\\ \frac{1}{t_R} &= \frac{AB}{t}, \tag{25.79}\\ h_R &= A^{-1}B^{-1/2}h, \tag{25.80}\end{align}$$

implying a renormalizability of the theory in terms of the two renormalization constants:

$$\begin{aligned}Z_t &= AB,\\ Z_\pi &= B.\end{aligned} \tag{25.81}$$

25.4 CRITICAL BEHAVIOUR IN 2+ϵ DIMENSIONS

Just as in the φ^4-theory where we studied the renormalization group in $4-\epsilon$ dimensions, we shall now consider $2+\epsilon$ dimensions for $\epsilon > 0$. The naive scale dimension of t is $\mu^{-\epsilon}$, where μ is a mass. We therefore go over to a dimensionless renormalized temperature by replacing in Eq. (25.52)

$$\frac{1}{t_R} \to \frac{\mu^\epsilon}{t_R}. \tag{25.82}$$

Then the renormalization equations for t_R reads

$$\frac{\mu^\epsilon}{t_R} = \frac{1}{t} - (N-2)L = \frac{1}{t}Z_t. \tag{25.83}$$

We now calculate L in $2+\epsilon$ dimensions. According to Eqs. (9.137) and (9.135), the integral diverges near $\epsilon = 0$ as follows

$$\begin{aligned} L = \int \frac{d^D q}{(2\pi)^D} \frac{1}{q^2+h} &= \bar{S}_D \frac{1}{2} \Gamma\left(1+\frac{\epsilon}{2}\right) \Gamma\left(-\frac{\epsilon}{2}\right) h^{\epsilon/2} \\ &= -\bar{S}_D \frac{1}{\epsilon} h^{\epsilon/2} + \mathcal{O}(\epsilon^1). \end{aligned} \tag{25.84}$$

We use once more the mass scale μ and remove from this integral the divergent expression

$$L_{div} = -\bar{S}_D \mu^{\epsilon} \frac{1}{\epsilon}. \tag{25.85}$$

Then (25.84) can be written

$$\frac{\mu^{\epsilon}}{t_R} = \frac{1}{t} + \frac{1}{2}(N-2)\bar{S}_D \mu^{\epsilon}, \tag{25.86}$$

or

$$t = \mu^{-\epsilon} t_R \left[1 + \frac{1}{\epsilon}(N-2)\bar{S}_D t_R\right] \tag{25.87}$$

From (25.86) we calculate the β-function

$$\beta(t_R) \equiv t_R^{-1} \mu\partial_\mu t_R = -t_R^2\, \mu\partial_\mu t_R^{-1}|_{t,\epsilon} = \epsilon t_R - (N-2)\bar{S}_D t_R^2 + \dots\ . \tag{25.88}$$

This has an ultraviolet-stable fixed point at

$$t_R^c = \frac{\epsilon}{(N-2)} + \dots \tag{25.89}$$

25.5 CRITICAL EXPONENTS

We now use the above results to calculate the critical exponents at the one-loop level. We first consider the exponent ν governing the way in which the correlation length ξ goes to infinity as t_R approaches the critical point t_R^c from above:

$$\xi \propto (t_R - t_R^c)^{-\nu}. \tag{25.90}$$

The following analysis is very similar to that in Chapter 21, except for one important difference: the physical variable which depends directly on the temperature of the system is now $t_R(\mu)$. In the φ^4-theory it was $m^2(\mu) \propto T/T_c - 1 \equiv \tau$. By analogy, we set here $\tau = t/t_c - 1$, ao that the behavior (25.90) amounts to $\xi \propto \tau^{-\nu}$.

The most direct way to calculate the critical exponent ν is based on the observation that physically observable quantities cannot have anomalous dimensions. Since the coherence length ξ is such a quantity, it satisfies $\mu\partial_\mu \xi(t) = 0$, and after expressing $\xi(t)$ in terms of μ in terms of the renormalized temperature t_R, which depends itself on μ, we obtain the renormalization group equation analog of the renormalization group equation (21.34) without a γ-term (recall Eq. (25.18)

$$\left[\mu\partial_\mu + \beta(t_R)\frac{\partial}{\partial t_R}\right]\xi(t_R,\mu) = 0, \tag{25.91}$$

this being an analog of the renormalization group equation (21.34) without the γ-terms. Now, dimensional analysis implies that ξ must depend on the two arguments as follows

$$\xi(t_R,\mu) = \mu^{-1}\bar{\xi}(t_R), \tag{25.92}$$

so that for $\bar{\xi}(t_R)$, the differential equation becomes

$$\left[-1 + \beta(t_R)\frac{\partial}{\partial t_R}\right]\bar{\xi}(t_R) = 0. \tag{25.93}$$

This is solved by

$$\bar{\xi}(t_R) = \text{const} \times \exp\left\{\int_0^{t_R} dt\, \frac{1}{\beta(t)}\right\}. \tag{25.94}$$

We may choose the correlation length ξ at zero temperature to coincide with μ^{-1}, which amounts to the initial condition

$$\bar{\xi}(0) = 1. \tag{25.95}$$

The integral is singular at $t = 0$, and a subtraction is necessary to extract a finite result. For this we make use of the explicit form of the singularity, $\beta(t) \approx 1/\epsilon t$ fund in (25.84), and rewrite (25.94) as follows

$$\bar{\xi}(t_R) = \text{const} \times t_R^{1/\epsilon} \exp\left\{\int_0^{t_R} dt \left[\frac{1}{\beta(t)} - \frac{1}{\epsilon t}\right]\right\}. \tag{25.96}$$

For $t_R \longrightarrow t_R^c$, this equation behaves like

$$\begin{aligned}\bar{\xi}(t_R) &\approx \text{const} \times (t_R^c)^{1/\epsilon} \exp\left\{\int_0^{t_R} dt \frac{1}{\beta'(t_R^c)(t - t_R^c)}\right\}\\ &\approx \text{const} \times (t_R^c)^{1/\epsilon}(t_R - t_R^c)^{1/\beta'(t_R^c)}.\end{aligned} \tag{25.97}$$

From this we identify the critical exponent of the coherence length as

$$\nu = -1/\beta'(t_R^c). \tag{25.98}$$

In Eq. (25.88) we found

$$\beta'(t_R^c) = \epsilon Z(N-2)S_D t_R, \tag{25.99}$$

which is equal to $-\epsilon$ at $t_R = t_R^c$. Thus

$$\nu = \epsilon^{-1}. \tag{25.100}$$

This result is independent of N, which is the reason why it coincides the exact result for $N \to \infty$ found in Chapter 17. This is to be compared with the O(N)-symmetric φ^4-theory where we obtained in $4 - \epsilon_\varphi$ dimensions [recall Eq. (21.189)]

$$\nu = \frac{1}{2} + \frac{N+2}{4(N+8)}\epsilon_\varphi. \tag{25.101}$$

The relation between the two expansion parameters ϵ is $\epsilon = 2 - \epsilon_\varphi$. Since both models describe the same physical system, they should have the same critical exponents. However, the expressions (25.98) and (25.101) have quite a different N-dependence. This shows that none of the two results can really be trusted in three dimensions. Apparantely, the parameter $\epsilon = 1$ is too large in either case to justify using the lowest-order term in the ϵ-expansion.

Let us calculate the critical exponent β of the spontaneous magnetization M in the ordered phase. It is defined by the power law in which the renormalized expectation of the field $\sigma = \sqrt{1 - \pi^2}$ goes to zero as t_R approaches the critical point [recall Eq. (21.157)]:

$$M \equiv \langle \sigma_R \rangle \equiv \Sigma_R \propto (-\tau)^\beta; \qquad t_R \to t_R^c - 0 \tag{25.102}$$

Since $\sigma = \sqrt{1 - \pi^2}$ has obviously a vanishing engeneering dimension, the magnetization $M = \sigma$ can depend only on $t_R(\mu)$. Moreover, due to the O(N)-symmetry, Σ is renormalized in the same way as Π in Eq. (25.45), so that

$$\Sigma_R = Z_\pi^{1/2} \sigma \tag{25.103}$$

Explicitly, this follows from Eq. (25.76). There the field Σ has gone over into into $\sqrt{B - \Pi_a^2}$ which is $B^{-1/2}\sqrt{1 - \Pi_{Ra}^2}$, thus confirming (25.103) [recalling (25.81)].

Writing the magnetization $M(t_R, \mu)$ as $M(t_R(\mu))$, we see that it satisfies the renormalization equation

$$\left[\beta(t_R)\frac{\partial}{\partial t_R} + \gamma_\pi(t_R)\right] M(t_R) = 0 \tag{25.104}$$

where

$$\gamma_\pi(t_R) = Z_\pi^{-1/2} \mu \partial_\mu Z_\pi^{1/2}. \tag{25.105}$$

According to (25.50) and (25.86), the lowest-order result is

$$\gamma_\pi(t_R) = \frac{(N-1)}{2S_D t_R}. \tag{25.106}$$

Equation (25.104) is then solved by

$$M(t_R) = \exp\left[-\int_0^t dt \frac{\gamma_\pi(t')}{\beta(t')}\right]. \tag{25.107}$$

Near the critical point t_R^c, this behaves like

$$M(t_R) \sim (-\tau)^{-\gamma_\pi(t_R^c)/\beta'(t_R^c)} \sim \xi^{-\gamma_\pi(t_R^c)}, \tag{25.108}$$

Recalling the definition (21.166) we identify the the critical exponent of spontaneous magnetization [not to be confused with the β-function (25.88)] as

$$\beta = \frac{\gamma_\pi\left(t_R^c\right)}{\beta'\left(t_R^c\right)}. \tag{25.109}$$

We shall denote $\gamma_\pi(t_R^c)$ and $\beta'(t_R^c)$ by γ^* and β'^*, respectively, so that $\beta = -\gamma^\pi/\beta'^*$. Inserting the lowest-order ϵ-expansions, $\gamma^* \approx (N-1)\epsilon/2, \quad \beta'^* \approx -\epsilon/(N-2)$, we obtain

$$\beta = \frac{N-1}{2(N-2)} + \mathcal{O}(\epsilon) \tag{25.110}$$

This is to be compared with the β-exponent of the O(N)-symmetric φ^4-theory. Takong the scaling expression (21.167) and inserting $D = 4 - \epsilon_\varphi, \quad \nu \approx 1/2 + \mathcal{O}(\epsilon_\varphi), \quad \eta \approx \mathcal{O}(\epsilon_\varphi^2)$] we see that

$$\beta = 1 + \mathcal{O}(\epsilon_\varphi) \tag{25.111}$$

Only the $N = \infty$ -values agree with each other, the low-N exponents are quite different, indicating again that in three dimensions, $\epsilon = \epsilon_\varphi = 1$ is somewhat too large in either expansion.

Let us finally calculate the anomalous dimension of the fields. The renormalized two point function of π fields $G^{(2)}(p)$ satisfies the renormalization group equation

$$\left[\mu\partial_\mu + \beta(t_R)\frac{\partial}{\partial t_R} + 2\gamma^\pi\right] G^{(2)}(p, t_R, \mu) = 0. \tag{25.112}$$

This can be rewritten as

$$\left[\mu\frac{d}{d\mu} + 2\gamma_\pi\right] G^{(2)}(p, t_R(\mu), \mu) = 0 \tag{25.113}$$

with the "running coupling" constant satisfying

$$\left[\mu\frac{d}{d\mu} + 2\gamma_\pi\right] G^{(2)}(p, t_R(\mu), \mu) = 0 \tag{25.114}$$

with the "running coupling" constant satisfying

$$\mu \frac{d}{d\mu} t_R(\mu) = \beta(t_R). \tag{25.115}$$

The solution reads

$$G^{(2)}\left(p, t_R(\mu), \mu\right) = \exp\left[-2\int_\sigma^1 \frac{d\mu'}{\mu}\gamma_\pi(\mu')\right] G^{(2)}(p, t_R(\mu_1), \mu_1). \tag{25.116}$$

Near the critical point, this behaves like

$$G^{(2)}(p, t_R(\mu), \mu) \propto \left(\frac{\mu}{\mu_1}\right)^{-2\gamma_\pi^*} G^{(2)}(p, t_R^c, \mu_1). \tag{25.117}$$

We now observe that the Fourier transformed Green function

$$G^{(2)}(p) = \int d^D x e^{ipx} \langle \pi_R(x)\pi_R(0)\rangle \tag{25.118}$$

contains now field $\pi_R(x)$ with a vanishing naive dimensions. Then $G^{(2)}(p)$ has the naive dimension $-D$, in contrast to the case of an ordinary scalar field $\varphi(x)$ where the dimension of $G^{(2)}(p)$ is -2 for all D. Thus (25.117) becomes

$$G^{(2)}(p, t_R(\mu), \mu) \propto \left(\frac{\mu}{\mu_1}\right)^{-2\gamma_\pi^*+D} G^{(2)}(p\mu/\mu_1, t_R^c, \mu) \tag{25.119}$$

Going to the critical point, $t_R(\mu) = t_R^c$, we see that $G^{(2)}(p)$ has to behave like a pure power in

$$G^{(2)}(p, t_R^c, \mu) \propto p^{-D}(p/\mu)^{2\gamma_\pi^*}. \tag{25.120}$$

From this we extract the exponent of the critical correlation function

$$\eta = -\epsilon + 2\gamma_\pi^*, \tag{25.121}$$

so that to lowest order in ϵ:

$$\eta = \frac{\epsilon}{N-2} + O(\epsilon^2). \tag{25.122}$$

Recall that η is defined by the anomalous behaviour of the Green function in x space, i.e.

$$G^{(2)}(x) = \langle \pi_R(x)\pi_R(0)\rangle \sim \frac{1}{x^\eta} \tag{25.123}$$

corresponding to $G^{(2)}(p) \propto p^{\eta - D}$. This is in contrast to the general form for the O(N)-symmetric φ^4-theory in $4 - \epsilon_\varphi$ dimensions, where φ has the naive dimension

$(D-2)/2$ and $G^{(2)}(x) \sim x^{-(D-2+\eta)}$. In that theory, the exponent η was [recall Eq. (21.188)]

$$\eta = \frac{N+2}{2(N+8)}\epsilon_\varphi^2 + O(\epsilon_\varphi^3). \tag{25.124}$$

The different N-dependence of (25.122) and (25.124) show once again that in three dimensions, $\epsilon = \epsilon_\varphi = 1$ is somewhat too large for either expansion.

It should be realized that due to the vanishing naive dimensions of the Goldstone fields $\pi(x)$ for any D, all the scaling relations are different from those derived in Chapter 21 for the φ^4-theory. In order to find all scaling rules, we can start out from the renormalization group equation obeyed by the general N-point function

$$\left\{\mu\partial_\mu + \beta(t_R)\frac{\partial}{\partial t_R} + n\gamma_\pi(t_R) + \gamma_h(t_R)h_R\partial_{h_R}\right\}\Gamma^{(n)}(p, t_R, h_R, \mu) = 0 \tag{25.125}$$

where [compare with (21.30) and (21.33)]

$$\begin{aligned}
\gamma_h &\equiv \frac{h}{h_R}\mu\partial_\mu\frac{h_R}{h} = \frac{h}{h_R}\mu\partial_\mu\left(Z_t^{-1}Z_\pi^{1/2}\right)|_{t,h} \\
&= \frac{h}{h_R}\left[\mu\partial_\mu\left(\mu^{-\epsilon}\frac{t_R}{t}\right)Z_\pi^{1/2} + \frac{1}{2}Z_t^{-1}Z_\pi^{1/2}\mu\partial_\mu\log Z_\pi\right] \\
&= \frac{h}{h_R}\left\{\mu^{-\epsilon}Z_t^{-1}Z_\pi^{1/2}\left[-\epsilon + \frac{1}{t_R}\beta(t_R)\right] + Z_t^{-1}Z_\pi^{1/2}\gamma_\pi\right\} \\
&= h\left[-\epsilon + \frac{\beta(t_R)}{t_R} + \gamma_\pi\right].
\end{aligned} \tag{25.126}$$

Near the critical point where $\beta(t_R)$ vanishes, this implies

$$\frac{h_R(\mu)}{h_R(\mu_1)} \propto \left(\frac{\mu}{\mu_1}\right)^{\gamma_\pi^* - \epsilon}. \tag{25.127}$$

Together with

$$\mu\frac{d}{d\mu}t_R(\mu) \approx \beta'^* \times (t_R - t_R^c), \tag{25.128}$$

we have

$$t_R(\mu) - t_R^c \propto \left(\frac{\mu}{\mu_1}\right)^{\beta'^*} = \left(\frac{\mu}{\mu_1}\right)^{-1/\nu}, \tag{25.129}$$

from which we conclude that μ_1 goes to zero near the critical point as follows

$$\left(\frac{\mu}{\mu_1}\right) \propto \mu\,\xi. \tag{25.130}$$

This implies that $h_R(\mu_1)$ vanishes according to the relation

$$\frac{h_R(\mu)}{h_R(\mu_1)} \propto \xi^{-\nu(\gamma_\pi^*-\epsilon)} \propto (\mu\epsilon)^{\gamma_\pi^*-\epsilon} \tag{25.131}$$

The general vertex function $\Gamma^{(n)}$ satisfies therefore the scaling relation

$$\Gamma^{(n)}(p,t_R(\mu),h_R(\mu),\mu) = \exp\left\{-n\int_{\mu_1}^{\mu}\frac{d\mu'}{\mu'}\gamma_\pi(\mu')\Gamma^{(n)}(p,t_R(\mu_1)h_R(\mu_1),\mu_1)\right\}. \tag{25.132}$$

Since the naive dimension of $\Gamma^{(n)}$ and h_R are D and 2, respectively, we can rescale the right-hand side and get in the critical regime

$$\left(\frac{\mu_1}{\mu}\right)^{D+n\gamma_\pi^*}\Gamma^{(n)}\left(p\frac{\mu}{\mu_1},t_R^c,h_R(\mu_1)\left(\frac{\mu}{\mu_1}\right)^2,\mu\right), \tag{25.133}$$

thus arriving at a scaling relation

$$\Gamma^{(n)}(p,t_R,h_R,\mu) \approx \xi^{-D}(\mu\xi)^{n\gamma_\pi^*}\Gamma^{(n)}\left(p\xi,t_R^c,h_R(\mu)(\mu\xi)^{D-\gamma_\pi^*},\mu\right). \tag{25.134}$$

In a similar fashion we derive the scaling relation for the vertex functions in the presence of background fields Π and Σ [in analogy with (21.93) and (21.94)]. Since both fields appear O(N)-symmetrically, we can suppress one of them

$$\Gamma^{(n)}(p,t_R,(\mu),\Sigma(\mu),\mu) = \xi^{-D-n\gamma_\pi^*}\Gamma^{(n)}\left(p\mu\xi,t_R^c,\Sigma/\mu,\xi^{\gamma_\pi^*},\mu\right). \tag{25.135}$$

From this we may derive all critical exponents of the system, and relate them to γ_π^* and ν. The exponent β of magnetization calculated in (25.109) satisfies the scaling relations

$$\beta = \gamma_\pi^*\nu = \frac{\nu}{2}(D-2+\eta), \tag{25.136}$$

wich is the same as that derived in $4-\epsilon_\varphi$ -expansion in Eq. (21.167).

Let us also find the critical exponent α of the specific heat C [recall (21.148)]. Since $\Gamma^{(0)} \propto \xi^D \propto \tau^{D\nu}$, and C measures the second temperature derivative of $\Gamma^{(0)}$ we see that

$$\alpha = D\nu - 2 \tag{25.137}$$

just as before in (25.112).

The critical exponent γ of the susceptibility [see (21.155)] is obtained by differentiating $\Gamma^{(0)}$ twice with respect to the field strength

$$\xi^{-1} \propto \frac{\partial^2\Gamma^{(0)}}{\partial\Sigma^2} \propto \xi^{-D+2\gamma_\pi^*} \propto \tau^{-\nu(2\gamma_\pi^*-D)}. \tag{25.138}$$

Hence

$$\gamma = \nu(2\gamma_\pi^* - D) = \nu(\eta - 2) \tag{25.139}$$

as before in (21.156). Alternatively, we could have used $\xi \propto d^2\Gamma^{(0)}/dh_R^2$, with the same result.

For the exponent δ of the critical magnetization [see [21.157)], we differentiate $\Gamma^{(0)}$ with respect to Σ and see that h_R must behave like

$$h_R \propto \frac{\partial\Gamma^{(0)}}{\partial\Sigma} \propto \xi^{-D+\gamma_\pi^*}(\Sigma\,\xi^{\gamma_\pi^*})^\delta. \tag{25.140}$$

If this relation is to remain nontrivial for $\tau \to 0$, we have the condition

$$-D + \gamma_\pi^* + \gamma_\pi^*\,\delta = 0, \tag{25.141}$$

or

$$\delta \;=\; -1 + \frac{D}{\gamma_\pi^*} = \frac{D+2-\eta}{D-2+\eta}, \tag{25.142}$$

just as in (21.160). The same critical exponent would of course follow from the relation

$$\Sigma_R \propto \frac{\partial h^0}{\partial h_R} \sim h_R^{1/\delta}. \tag{25.143}$$

Thus, even though the derivation was completely different, all scaling relations are exactly the same as those found in the O(N)-symmetric φ^4-theory. The basic reason is that since $\xi^{\gamma_\pi^*} \propto \tau^\beta$ and $\xi^{-D+\gamma_\pi^*}, \propto \tau^{\delta\beta}$, the equation of state

$$\begin{aligned} j \;&=\; \xi^{-D+\gamma_\pi^*}\, v'(t_R^c, \Sigma\,\xi^{\gamma_\pi^*}, \mu) \\ &=\; \tau^{\delta\beta} f\left(\frac{\Sigma}{\tau^\beta}\right) \end{aligned} \tag{25.144}$$

follows Widom's general scaling form (21.176)

$$\frac{h}{M^\delta} = f\left(\frac{\tau}{M^{1/\beta}}\right) \tag{25.145}$$

25.6 TWO- AND THREE-LOOP RESULTS

For completeness, let us also write down the result up to the three loop level. The two-loop diagrams are shown in Fig. 25.1. We have omitted the corresponding diagrams involving the $1/a^D$ terms, for brevity. The three loop diagrams are quite numerous. In order to display them we drop the dashed and wiggly lines and show only the topological structure in Fig. 25.2. The two renormalization constants have the following $1/\epsilon$-singularities

$$\begin{aligned} Z_t &= 1+\frac{N-2}{\epsilon}t_R+\left[\frac{(N-2)^2}{\epsilon^2}+\frac{N-2}{2\epsilon}\right]t_R^2 \\ &\quad +\left[\frac{(N-2)^3}{\epsilon^3}+\frac{7}{6}\frac{(N-2)^2}{\epsilon^2}+\frac{(N-2)(N+2)}{12\epsilon}\right]t_R^3+\dots\,, \end{aligned} \tag{25.146}$$

$$\begin{aligned} Z_\pi &= 1+\frac{N-1}{\epsilon}t_R+\frac{(N-1)(N-\frac{3}{2})}{\epsilon^2}t_R^2 \\ &+\left[-\frac{N-1}{3\,\epsilon^3}\left(-3N^2+\frac{19}{2}N-\frac{15}{2}\right)+\frac{(N-1)(N-2)}{3\epsilon^2}+\frac{(N-2)(N-1)}{4\epsilon}\right]t_R^3+\dots\,. \end{aligned} \tag{25.147}$$

From this one finds the functions $\beta(t_R)$ and $\gamma_\pi(t_R)$ [recalling (25.88) and (25.105)]

$$\begin{aligned} \beta(t_R) &= \frac{\epsilon t_R}{1+t_R\frac{\partial}{\partial t_R}\log Z_t} \\ &= \epsilon t_R-(N-2)t_R^2-(N-2)t_R^3-\frac{1}{4}(N-2)(N+2)t_R^4+\dots\,, \\ 2\gamma_\pi(t_R) &= \beta(t_R)\frac{d\log Z_\pi}{dt_R} = (N-1)t_R+\frac{3}{4}(N-1)(N-2)t_R^3+\dots\,. \end{aligned} \tag{25.148}$$

The critical coupling t_R^c defined by $\beta(t_R^c)=0$ has the ϵ-expansion

$$t_R^c=\frac{\epsilon}{N-2}-\frac{\epsilon^2}{(N-2)^2}+\frac{6-N}{4}\frac{\epsilon^3}{(N-2)^2}+\dots\,, \tag{25.149}$$

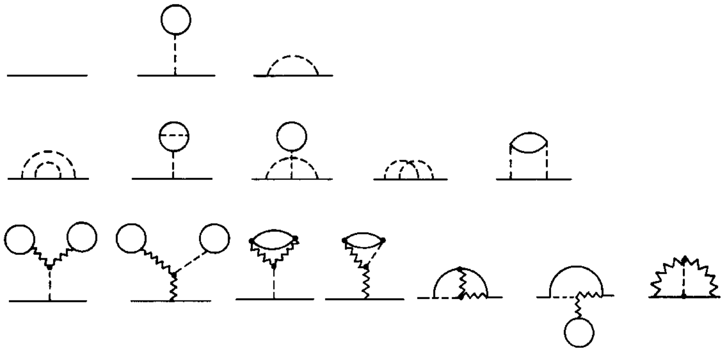


FIGURE 25.1 Two-loop diagrams

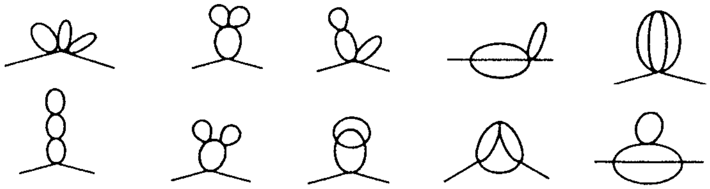


FIGURE 25.2 Three-loop diagrams

and the critical exponents are

$$\nu^{-1} = -\beta'(t_R^c) = \epsilon + \frac{\epsilon^2}{N-2} + \frac{\epsilon^3}{2(N-2)} + \dots\,, \tag{25.150}$$

$$\eta = -\epsilon + 2\gamma_\pi(t_R^c) = \frac{\epsilon}{N-2} - (N-1)\frac{\epsilon^2}{(N-2)^2} + \frac{N(N-1)}{2}\frac{\epsilon^3}{(N-2)^3} + \dots \tag{25.151}$$

From the scaling law $\beta = \nu(D-2+\eta)/2$ we obtain the critical exponent magnetization

$$\beta = \frac{N-1}{2(N-2)} - \frac{(N-1)}{(N-2)^2}\epsilon + \frac{3}{2}\frac{N-1}{(N-2)^3}\epsilon^2 + \dots \tag{25.152}$$

These ϵ-expansion show a very poor convergence at $\epsilon = 1$, where they are supposed to describe the three-dimensional situation. Moreover, the series for ν^{-1} has no alternating signs, indicating that it may not even be Borel-summable. One might nevertheless attempt a Borel-Padé resummation.

Consider, for example, the case of $N = 3$ (vector model) where

$$\nu^{-1} = \epsilon + \epsilon^2 + \frac{1}{2}\epsilon^3 + \dots\,. \tag{25.153}$$

It is the Borel transformation of the function

$$B_\nu(t) = \epsilon t + \epsilon^2\frac{t^2}{2!} + \epsilon^3\frac{t^3}{2\cdot 3!} + \dots\,, \tag{25.154}$$

i.e.

$$\nu^{-1} = \int_0^\infty e^{-t} B_\nu(t). \tag{25.155}$$

Let us take a simple [1, 2]-Padé approximation for $B_\nu(t)$. This is a ratio of a polynomial of degree one in the numerator and of degree two in the denominator, which has the same small-t expansion as in (25.154). It reads

$$B_\nu(t) = \frac{\epsilon t}{1 - \frac{\epsilon}{2}t + \frac{\epsilon^2}{6}t^2}, \tag{25.156}$$

and it is easy to verify that it has the expansion (25.153). Inserted into (25.155) we obtain at $\epsilon = 1$:

$$\nu^{-1} = \int_0^\infty e^{-t}\frac{t}{1 - \frac{t}{2} + \frac{t^2}{6}} \approx 1.25. \tag{25.157}$$

Note that the [1, 1] approximant would have a pole for $t > 0$ preventing its use.

To resum similarly the series (25.151) for η, we may use a [2,1] Padè-approximation:

$$\begin{aligned} B_\eta(t) &= \epsilon t - \frac{2\epsilon^2 t^2}{2!} + 3\epsilon^3 \frac{t^3}{3!} + \dots \\ &= \epsilon t \frac{1-\epsilon t/2}{1+\epsilon t/2}, \end{aligned} \tag{25.158}$$

to find at $\epsilon = 1$:

$$\eta = \int_0^\infty e^{-t} t \frac{1-t/2}{1+t/2} = 0.11. \tag{25.159}$$

These results may be compared with the well-known critical exponents of the three-dimensional classical Heisenberg model:

$$\nu^{-1} \approx 1.39, \tag{25.160}$$

$$\eta \approx 0.04. \tag{25.161}$$

The numbers for ν^{-1} agree reasonably well with each other considering the arbitrariness of the resummation procedure. The numbers for η agree insofar as that both are small.

Recently, the ϵ-expansions have been driven to order ϵ^4 with an entirely different technique using perturbation expansions in $1/N$.[1] These results for the forth-order contributions to the series (25.150) and (25.151) are

$$\nu_4^{-1} = -\left[30 - 14 + n^2 + (54 - 18n)\zeta(3)\right] \frac{\epsilon^4}{4(n-2)^3}, \tag{25.162}$$

$$\eta_4 = -(n-1)\left[-6 + 2N + n^2 + (-12 + n + n^2)\,\zeta(3)\right] \frac{\epsilon^4}{4\,(n-2)^4}. \tag{25.163}$$

The additional terms do not improve the critical exponents if only Padé-Borel resummation techniques are used. Another pmore powerful method is needed to extract precise numbers.

25.7 VARIATIONAL RESUMMATION OF ϵ-EXPANSIONS

Having seen the difficulties in extracting accurate critical exponents from the above ϵ-expansions, we decide to resum the above series using information from the $4-\varepsilon$-expansions of the ϕ^4-theories. This becomes possible by rewriting the latter as power series in the variable $\tilde{\varepsilon} \equiv 2(4-D)/(D-2)$. The initial five expansion coefficients of these functions are known from ε-expansions of critical exponents in O(N)-symmetric ϕ^4-theory in $D = 4 - \varepsilon$ dimensions. The first four expansion coefficients of the strong-coupling expansions are determined from (25.150), (25.151), (25.162), and (25.163). Recall that the critical exponent ν of the classical Heisenberg model with $N = 3$, which governs the divergence of the coherence length as $\xi \propto |T - T_c|^{-\nu}$, the renormalization group treatment of seven-loop expansions in three dimensions yields $\nu = 0.7073 \pm 0.0030$,[2] whereas five-loop expansions in $D = 4 - \varepsilon$ dimensions [3] extrapolated to $\varepsilon = 1$. lead to $\nu = 0.7050 \pm 0.0055$[3]. Apart from the expansion coefficients, the latter results incorporate information on the large-order growth contained in the tip of the left-hand cut in the complex coupling-constant plane. Results very close to these were recently obtained from a novel strong-coupling ϕ^4-theory[4] using the six-loop expansions available in the literature.

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[1] W. Bernreuther and F.J. Wegner, Phys. Rev. Lett. **57**, 1383 (1986); I. Jack, D.R.T. Jones, and N. Mohammedi, Phys. Lett. B **220**, 171 (1989), Nucl. Phys. B **322**, 431 (1989); N.A. Kivel, A.A. Stepanenko, A.N. Vasil'ev, Nucl.Phys. B **424**, 619 (1994) (hep-th/9308073).

It is generally accepted that, as a consequence of the *universality hypothesis* of critical phenomena of all systems with equal Goldstone bosons, the same critical exponents should be obtainable from renormalization group studies of O(N) nonlinear σ-models in $D = 2 + \epsilon$ dimensions at $\epsilon = 1$, unless the second-order character of the transition is destroyed by fluctuations. The fact that the latter expansions have remained, up to now, rather useless for any practical calculation due to their non-Borel character has led some authors to doubt the use of such expansions around the lower critical dimension altogether[5]. This would be quite unfortunate, since it would jeopardize other intreresting theories such as Anderson's theory of localization[6]. Basis of these doubts is the increasing relevance of higher powers of the derivative term.[7] Hopes for the utility of these expansions are however not completely lost, since the argument involves an interchange of limits of continuing in ϵ and of increasing the number of derivatives.[8].

In this Section we can confirm these hopes by extracting from the series (25.150), (25.151), (25.162), and (25.163) supplemented by the five-lopp ε-expansions around four dimensions very accurate critical exponents ν for the classical Heisenberg model as well as for the universality classes O(N) with $N = 0, 1, 2$.

When evaluated the series for ν^{-1} at $\epsilon = 1$, the first series yields for the three-dimensional O(3)-model the diverging successive values $\nu^{-1} = (1,\ 2,\ 2.5\ , 3.25)$. Also Padé approximations do not help, the best of them, the [1,2]-approximation, giving the too large value $\nu = 2$. So far, the only result which is not far from the true value has been obtained via the Padé-Borel transform [9]

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[2] R. Guida and J. Zinn-Justin, preprint (cond-mat/9803240). This paper paper uses unpublished expansions of the renormalization group functions in three dimensions up to seven loops by D.B. Murray and B.G. Nickel.

[3] H. Kleinert, J. Neu, V. Schulte-Frohlinde, K.G. Chetyrkin, and S.A. Larin, Phys. Lett. B *272*, 39 (1991) (hep-th/9503230), Erratum ibid. B *319* (1993). See also H. Kleinert and V. Schulte-Frohlinde, Phys. Lett. *B342*, 284 (1995) (cond-mat/9503038).

[4] H. Kleinert, Phys. Rev. D *57*, 2264 (1998) (E-Print aps1997jun25_001); addendum (cond-mat/9803268); See also (cond-mat/9801167).

[5] G.E. Castilly and S. Chakravarty, *Is the phase transition of the Heisenberg model described by the* $(2+\epsilon)$*-expansion of the Nonlinear* σ*-model?* Nucl Phys B *485*, 613 (1997) (cond-mat/9605088).

[6] P.W. Anderson, Phys. Rev. *109*, 1429 (1958).

[7] F. Wegner, Z. Phys. B *78*, 36 (1990).

[8] E. Brézin and S. Hikami (cond-mat/9612016).

$$P^{[1,2]}(\epsilon, t) = \frac{\epsilon t}{1 - \epsilon t/2 + \epsilon^2 t^2/6}, \tag{25.164}$$

from which one obtains the ϵ-dependent critical exponent

$$\nu^{-1}(\epsilon) = \int_0^\infty dt\, e^{-t} P^{[1,2]}(\epsilon, t) \tag{25.165}$$

whose value at $\epsilon = 1$ is ≈ 1.252, corresponding to $\nu \approx 0.799$, still too large to be useful. The other Padé-Borel approximants are singular and thus of no use, as shown in Fig. 25.3.

The full ϵ-dependence of the power series (25.162) and the Padé-Borel-approximation (25.165) can be seen in Fig. 25.4.

A direct evaluation of the series for the anomalous dimension η yields the successive the even worse values (2, -2, 4, -5). Here the nonsingular Borel-Padé approximations $[2,1]$, $[1,2]$, and $[1,1]$ yield 0.147, 0.150, and 0.139, rather than the correct value 0.032. The full ϵ-dependence of the power series (25.163) and the Padé[2,1]-Borel-approximation are also shown in Fig. 25.4.

25.7.1 Strong-Coupling Theory

The remedy for these problems comes from our theory developed in the reference quoted in Footnote 4 which allows us to extract the strong-coupling properties of a ϕ^4-theory from perturbation expansions. In particular, we found power behavior for the renormalization constants at large couplings, and from this all critical exponents of the system. By using the known expansion coefficients of the renormalization constants in three dimensions up to six loops, we derived extremely accurate values for the critical exponents. The method is a systematic extension to arbitrary orders[9] of the Feynman-Kleinert variational approximation to path integrals.[10] For an anharmonic oscillator, this so-called *variational perturbation theory*[11] yields expansions which converge uniformly in the coupling strength and exponentially fast, like $e^{-\text{const}\times L^{1/3}}$ in the order L of the approximation, as was observed in various works[12] and proved recently.[13]. The extension to field theory showed to same type of convergence, with the power $1/3$ replaced by $1-\omega$, where ω is the critical exponent governing the approach to scaling. This field-theoretic development will now be combined with an earlier interpolation procedure[14] to resum the non-Borel expansion (25.150) and (25.162).

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[9] H. Kleinert, Phys. Lett. A **173**, 332 (1993) (www.physik. fu-berlin.de/~kleinert/kleiner_re3.html#213).

[10] R.P Feynman and H. Kleinert, Phys. Rev. **A34**, 5080 (1986) (www.physik.fu-berlin.de/~kleinert/kleiner_re2.html#159).

[11] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics,* World Scientific, Singapore 1995, Second extended edition, pp. 1–850 (www.physik.fu-berlin.de/~kleinert/kleiner_re.html#b5)

[12] W. Janke and H. Kleinert, Phys. Lett. **A199**, 287 (1995), Phys. Rev. Lett. **75**, 2787 (1995) (quant-ph/9502019).

[13] H. Kleinert and W. Janke, Phys. Lett. **A206**, 283 (1995) (quant-ph/9509005). A convergence proof for the anharmonic oscillator which is completely equivalent our results in [16] was given by R. Guida, K. Konishi, and H. Suzuki, Annals Phys. **249**, 109 (1996) (hep-th/9505084).

Let us briefly recall the interpolation procedure by which a divergent weak-coupling expansion of the type $E_L(g_0)=\sum_{n=0}^{L} a_n g_0^n$ can be combined with a strong-coupling expansion $E_M(g_0)=g_0^{p/q}\sum_{m=0}^{M} b_m (g_0^{-2/q})^m$. Previously treated examples [18] were the anharmonic oscillator with parameters $p=1/3,\ q=3$ for the energy eigenvalues, and the Fröhlich polaron with $p=1,\ q=1$ for the ground-state energy and $p=4,\ q=1$ for the mass. As described in detail in the textbook in Footnote 11, the first step is to rewrite the weak-coupling expansion with the help of an auxiliary scale parameter κ as

$$E_L(g_0)=\kappa^p\sum_{n=0}^{L} a_n\left(\frac{g_0}{\kappa^q}\right)^n \tag{25.166}$$

where κ is eventually set equal to 1. We shall see below that the quotient p/q parametrizes the *leading power behavior* in g_0 of the strong-coupling expansion, whereas $2/q$ characterizes the *approach* to the leading power behavior. In a second step we replace κ by the identical expression

$$\kappa \rightarrow \sqrt{K^2+\kappa^2-K^2} \tag{25.167}$$

containing a dummy scaling parameter K. The series (25.166) is then reexpanded in powers of g_0 up to the order L, thereby treating κ^2-K^2 as a quantity of order g_0. The result is most conveniently expressed in terms of dimensionless parameters $\hat{g}_0\equiv g_0/K^q$ and $\sigma\equiv(1-\hat{\kappa}^2)/\hat{g}_0$, where $\hat{\kappa}\equiv\kappa/K$. Then the replacement (25.167) amounts to

$$\kappa \longrightarrow K(1-\sigma\hat{g}_0)^{1/2}, \tag{25.168}$$

so that the reexpanded series reads explicitly

$$W_L(\hat{g}_0,\sigma)=K^p\sum_{n=0}^{L}\varepsilon_n(\sigma)\,(\hat{g}_0)^n\,, \tag{25.169}$$

with the coefficients:

$$\varepsilon_n(\sigma)=\sum_{j=0}^{n} a_j\begin{pmatrix}(p-qj)/2\\ n-j\end{pmatrix}(-\sigma)^{n-j}. \tag{25.170}$$

For any fixed g_0, we form the first and second derivatives of $W_L(g_0,K)$ with respect to K, calculate the K-values of the extrema and the turning points, and select the smallest of these as the optimal scaling parameter K_L. The function $W_L(g_0)\equiv W_L(g_0,K_L)$ constitutes the Lth variational approximation $E_L(g_0)$ to the function

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[14] H. Kleinert, Phys. Lett. A **207**, 133 (1995) (quant-ph/9507005).

$E(g_0)$. It is easy to take this approximation to the strong-coupling limit $g_0 \to \infty$. For this we observe that (25.169) has the scaling form

$$W_L(g_0, K) = K^p w_L(\hat{g}_0, \hat{\kappa}^2). \tag{25.171}$$

For dimensional reasons, the optimal K_L increases with g_0 like $K_L \approx g_0^{1/q} c_L$, so that $\hat{g}_0 = c_L^{-q}$ and $\sigma = 1/\hat{g}_0 = c_L^q$ remain finite in the strong-coupling limit, whereas $\hat{\kappa}^2$ goes to zero like $1/[c_L(g_0/\kappa^q)^{1/q}]^2$. Hence

$$W_L(g_0, K_L) \approx g_0^{p/q} c_L^p w_L(c_L^{-q}, 0). \tag{25.172}$$

Here c_L plays the role of the variational parameter to be determined by the optimal extremum or turning point of $c_L^p w_L(c_L^{-q}, 0)$. The full strong-coupling expansion is obtained by expanding $w_L(\hat{g}_0, \hat{\kappa}^2)$ in powers of $\hat{\kappa}^2 = (g_0/\kappa^q \hat{g}_0)^{-2/q}$. The result is

$$W_L(g_0) \;=\; g_0^{p/q}\left[\, b_0(\hat{g}_0) + b_1(\hat{g}_0)\left(\frac{g_0}{\kappa^q}\right)^{-2/q} + b_2(\hat{g}_0)\left(\frac{g_0}{\kappa^q}\right)^{-4/q} + \ldots\right] \tag{25.173}$$

with

$$b_n(\hat{g}_0) = \frac{1}{n!} w_L^{(n)}(\hat{g}_0, 0)\hat{g}_0^{(2n-p)/q}\,, \tag{25.174}$$

where $w_L^{(n)}(\hat{g}_0, \hat{\kappa}^2)$ is the nth derivatives of $w_L(\hat{g}_0, \hat{\kappa}^2)$ with respect to $\hat{\kappa}^2$. Explicitly:

$$\frac{1}{n!} w_L^{(n)}(\hat{g}_0, 0) = \sum_{l=0}^{L} (-1)^{l+n} \sum_{j=0}^{l-n} a_j \binom{(p-qj)/2}{l-j} \binom{l-j}{n} (-\hat{g}_0)^j. \tag{25.175}$$

The optimal expansion of the energy (25.173) is obtained by expanding

$$\hat{g}_0 = \gamma_0 + \gamma_1 \left(\frac{g_0}{\kappa^q}\right)^{-2/q} + \gamma_2 \left(\frac{g_0}{\kappa^q}\right)^{-4/q} + \ldots\,, \tag{25.176}$$

where $\gamma_0 = c_L^{-q}$, and finding the optimal extremum (or turning point) in the resulting polynomials of $\gamma_1, \gamma_2, \ldots$. In this way we obtain a systematic strong-coupling coupling expansion in powers of $(g_0/\kappa^q)^{-2/q}$. This is done as follows: We first optimize the leading strong-coupling coefficient $b_0(\hat{g}_0)$ in $\hat{g}_0$, and identify the optimal position by γ_0. Optimizing $W_L(g_0)$ with the expansion (25.176), in $\gamma_1, \gamma_2, \ldots$, yields for the parameters $p = -2, q = 2$ at the coefficients $\gamma_1, \gamma_2, \ldots$ and optimal $b_n(\hat{g}_0)$'s by the equations listed in Table 25.1.

It was demonstrated in [18] how one can now find a variational perturbation series for functions for which one knows L weak-coupling and M strong-coupling expansion coefficients. We must merely extend the set of of coefficients $a_1, \ldots, a_L$ by M unknown ones $a_{L+1}, \ldots, a_{L+M}$, and determine the latter via a fit of the resulting strong-coupling coefficients $b_0, \ldots, b_{M-1}$ to the known ones.

25.7.2 Interpolation

This interpolation procedure will now be applied to the perturbation expansion (25.162) in $2+\epsilon$ dimensions, considering it as the *strong-coupling expansion* of a series in the variable $\tilde{\varepsilon} = 2(4-D)/(D-2) = 4(1-\epsilon/2)/\epsilon = \varepsilon/(1-\varepsilon/2)$:

$$\begin{aligned}\nu^{-1} &= 4\tilde{\varepsilon}^{-1} - 8\frac{N-4}{N-2}\tilde{\varepsilon}^{-2} + 16\frac{N-4}{N-2}\tilde{\varepsilon}^{-3} \\ &\quad -32\left\{[52+108\zeta(3)] - [16+36\zeta(3)]N + N^2\right\}\frac{\tilde{\varepsilon}^{-3}}{(N-2)^3} + \dots \,. \qquad (25.177)\end{aligned}$$

The weak-coupling expansion of this series is [3]

$$\begin{aligned}\nu^{-1} &= 2 - \frac{N+2}{N+8}\tilde{\varepsilon} + \left(20+3N+N^2\right)\frac{(2+N)\tilde{\varepsilon}^2}{2(8+N)^3} \\ &+\left[-2240 - 624N - 212N^2 - 9N^3 - 2N^4 + 8\cdot 12(8+N)(22+5N)\zeta(3)\right]\frac{(2+N)\tilde{\varepsilon}^3}{8(8+N)^5} \\ &+\Big[5\left(568576 + 382144N + 103920N^2 + 9532N^3 + 1142N^4 + 21N^5 + 4N^6\right) \\ &+80\left(-249600 - 148960N - 42912N^2 - 6516N^3 - 350N^4 + 3N^5\right)\zeta(3) + 80\cdot 18(8+N)^3(22+5n)\zeta(4) \\ &-80\cdot 80(8+N)^2\left(186+55n+2n^2\right)\zeta(5)\Big]\frac{(2+N)}{160(8+N)^7}\tilde{\varepsilon}^4 \\ &+\Big[945\left(-105091072 - 106771456N - 47635968N^2 - 11768576N^3 - 1835504N^4 - 122812N^5 - 6270N^6 - 45N^7 - 8N^8\right) \\ &+15120\left(57911296 + 46323968N + 17913728N^2 + 3869024N^3 + 514592N^4 + 46900N^5 + 1902N^6 - 37N^7\right)\zeta(3) \\ &+15120\left(-47874048 - 40615936N - 11928064N^2 - 1525888N^3 - 89408N^4 - 3200N^5 - 128N^6\right)\zeta^2(3) \\ &+945\left(101376 + 61056N + 13392N^2 + 1278N^3 + 45N^4\right)\zeta(4) \\ &+256\cdot 945(8+N)^2\left(345552 + 193822N + 48749N^2 + 6506N^3 + 235N^4\right)\zeta(5) \\ &+945\cdot 56448(8+N)^3\left(526+189N+14N^2\right)\zeta(7)\Big]\frac{(N+2)\tilde{\varepsilon}^5}{120960(8+N)^9} + \dots\,, \qquad (25.178)\end{aligned}$$

whose numerical forms are for $N = 3,4,5,1$

$$N=3:\ \nu^{-1} = 2 - 0.45455\,\tilde{\varepsilon} + 0.071375\,\tilde{\varepsilon}^2 + 0.15733\,\tilde{\varepsilon}^3 - 0.52631\,\tilde{\varepsilon}^4 + 1.5993\,\tilde{\varepsilon}^5 \qquad (25.179)$$

$$N=4:\ \nu^{-1} = 2 - 0.5\,\tilde{\varepsilon} + 0.0833333\,\tilde{\varepsilon}^2 + 0.147522\,\tilde{\varepsilon}^3 - 0.499944\,\tilde{\varepsilon}^4 + 1.47036\,\tilde{\varepsilon}^5, \qquad (25.180)$$

$$N=5:\ \nu^{-1} = 2 - 0.538462\,\tilde{\varepsilon} + 0.0955849\,\tilde{\varepsilon}^2 + 0.135442\,\tilde{\varepsilon}^3 - 0.469842\,\tilde{\varepsilon}^4 + 1.34491\,\tilde{\varepsilon}^5, \qquad (25.181)$$

$$N=1:\ \nu^{-1} = 2 - 0.333333\,\tilde{\varepsilon} + 0.0493827\,\tilde{\varepsilon}^2 + 0.158478\,\tilde{\varepsilon}^3 - 0.539937\,\tilde{\varepsilon}^4 + 1.78954\,\tilde{\varepsilon}^5. \qquad (25.182)$$

Extending these series by four more terms $a_6\,\tilde{\varepsilon}^6 + a_7\,\tilde{\varepsilon}^7 + a_8\,\tilde{\varepsilon}^8 + a_9\,\tilde{\varepsilon}^9$, we calculate the strong-coupling coefficients (25.174) by extremizing (25.173) with (25.176), after identifying g_0 with $\tilde{\varepsilon}$ and the parameters (p,q) with $(-2,2)$. Then the coefficients a_6, a_7, a_8, a_9 are determined to make $b_0(\hat{g}_0), b_1(\hat{g}_0), b_2(\hat{g}_0), b_3(\hat{g}_0)$ agree with (25.183). The technique of doing this is described in detail in Ref. [18].

In order to see how the result improves with the number M of additional terms in (25.176), we go through this procedure successively for $M = 1,2,3,4$. The successive additional expansion coefficients for the O(N) universality classes with N = 3, 4, 5, 1 are listed in Tables 25.2–25.5, repsectively. The four resulting curves for $\nu^{-1}(\varepsilon)$ are shown in Figs. 25.4–25.7. For $N = 3$, the successive critical exponents ν at $\varepsilon = 1$ taken form Fig. 25.4 are $(\nu_1,\nu_2,\nu_3,\nu_4) =$

(0.87917, 0.75899, 0.731431, 0.712152). Their M-dependence is plotted in Fig. 25.8 as a function of the variable $x = M^{-2}$ which makes them lie approximately on a straight line intercepting the ν-axis at $\nu_\infty = 0.705$. This extrapolated value is in excellent agreement with the previous determination [4] from ϕ^4-theories, and somewhat smaller than the seven-loop result in [2]. The other O(N) universality classes are displayed analogously.

Since the ϵ-expansion (25.162) is singular at $N = 2$, we expect difficulties with our procedure for $N < 2$. Indeed, the determination of the expansion coefficients in Table 25.5 shows a large irregularity for $M = 3$, and the successive approximations for ν^{-1} in Fig. 25.7 show no sign of convergence with increasing M.

Finally, we plot our highest ($M = 4$) approximations for $N = 3$, 4, 5 together with the large-N approximations for $N = \infty$, 20, 10, 6 in Fig. 25.12 to see the trend for increasing N, which shows that the latter for $N = 6$ is still far from the exact curve. This can also be seen in Fig. 3 of Ref. [19].

The same calculation is done for the critical exponent η. In the variable $\tilde{\varepsilon}$, the series (25.163) reads

$$\begin{aligned}\eta &= \frac{\tilde{\varepsilon}^{-1}}{N-2} - 2n\frac{\tilde{\varepsilon}^{-2}}{(N-2)^2} + 8n(N-1)\frac{\tilde{\varepsilon}^{-3}}{(N-2)^3}\\ &\quad +16(N-1)\left[\left(6-2n^2\right)+\Big[12-n-n^2\Big)\zeta(3)\right]\frac{\tilde{\varepsilon}^{-4}}{(N-2)^4}+\dots \qquad (25.183)\end{aligned}$$

whereas the weak-coupling expansion is [3]

$$\begin{aligned}\eta/\epsilon^2 &= \frac{2+N}{2(N+8)^2} + \left(272+56\,N-N^2\right)\frac{(2+N)\;\epsilon}{8(N+8)^4}\\ &+\left\{46144+17920\,N+1124\,N^2-230\,N^3-5\,N^4-32\cdot 12\;(22+5\,N)\;\zeta(3)\right\}\frac{(2+N)\;\epsilon^2}{32(N+8)^6}\\ &+\Big\{5655552+2912768\,N+262528\,N^2-121472\,N^3-27620\,N^4-946\,N^5-13\,N^6\\ &+16(N+8)\;\left(-171264-68672\,N-1136\,N^2+1220\,N^3+10\,N^4+N^5\right)\zeta(3)\\ &+128\cdot 9\,(N+8)^3\;(22+5\,N)\;\zeta(4)+128\cdot 40\,(N+8)^2\left(186+55\,N+2\,N^2\right)\;\zeta(5)\Big\}\frac{(2+N)\;\epsilon^3}{128(N+8)^8}+\dots \qquad (25.184)\end{aligned}$$

whose numerical forms are for $N = 3, 4, 5, 1$

$$n=3:\;\; \eta/\epsilon^2 = 5/242\; + 0.0183987\,\tilde{\epsilon} - 0.0166488\,\tilde{\epsilon}^2 + 0.032432\,\tilde{\epsilon}^3, \qquad (25.185)$$

$$n=4:\;\; \eta/\epsilon^2 = 1/48\; + 0.0173611\,\tilde{\epsilon} - 0.0157657\,\tilde{\epsilon}^2 + 0.029057\,\tilde{\epsilon}^3, \qquad (25.186)$$

$$N=5:\;\; \eta/\epsilon^2 = 7/338\; + 0.0161453\,\tilde{\epsilon} - 0.0148734\,\tilde{\epsilon}^2 + 0.0259628\,\tilde{\epsilon}^3, \qquad (25.187)$$

$$N=1:\;\; \eta/\epsilon^2 = 1/54\; + 0.01869\,\tilde{\epsilon} - 0.0176738\,\tilde{\epsilon}^2 + 0.0386577\,\tilde{\epsilon}^3. \qquad (25.188)$$

Extending these series by four more terms $a_6\,\tilde{\varepsilon}^6 + a_7\,\tilde{\varepsilon}^7 + a_8\,\tilde{\varepsilon}^8 + a_9\,\tilde{\varepsilon}^9$, we calculate the strong-coupling coefficients (25.174) by extremizing (25.173) with (25.176), after identifying g_0 with $\tilde{\varepsilon}$ and the parameters (p, q) with $(-2, 2)$. Then the coefficients a_6, a_7, a_8, a_9 are determined to make $b_0(\hat{g}_0), b_1(\hat{g}_0), b_2(\hat{g}_0), b_3(\hat{g}_0)$ agree with (25.183). The technique of doing this is described in detail in Ref. [18].

In order to see how the result improves with the number M of additional terms in (25.176), we go through this procedure successively for $M = 1, 2, 3, 4$.

The successive additional expansion coefficients for the O(N) universality classes with N = 3, 4, 5, 1 are listed in Tables 25.2–25.5, repsectively. The four resulting curves for $\nu^{-1}(\varepsilon)$ are shown in Figs. 25.4–25.7. For N = 3, the successive critical exponents ν at $\varepsilon = 1$ taken form Fig. 25.4 are $(\nu_1, \nu_2, \nu_3, \nu_4) =$ (0.87917, 0.75899, 0.731431, 0.712152). Their M-dependence is plotted in Fig. 25.8 as a function of the variable $x = M^{-2}$ which makes them lie approximately on a straight line intercepting the ν-axis at $\nu_\infty = 0.705$. This extrapolated value is in excellent agreement with the previous determination [4] from ϕ^4-theories, and somewhat smaller than the seven-loop result in [2]. The other O(N) universality classes are displayed analogously.

Since the ϵ-expansion (25.162) is singular at $N = 2$, we expect difficulties with our procedure for $N < 2$. Indeed, the determination of the expansion coefficients in Table 25.5 shows a large irregularity for $M = 3$, and the successive approximations for ν^{-1} in Fig. 25.7 show no sign of convergence with increasing M.

Finally, we plot our highest ($M = 4$) approximations for N = 3, 4, 5 together with the large-N approximations for $N = \infty$, 20, 10, 6 in Fig. 25.12 to see the trend for increasing N, which shows that the latter for $N = 6$ is still far from the exact curve. This can also be seen in Fig. 3 of Ref. [19].

TABLE 25.1 Equations determining the coefficients $b_n(\hat{g}_0)$ in the strong-coupling expansion (25.173) and the associated $\gamma_i \equiv c_n^{-q}\delta_i$ in (25.176) from the functions $\bar{b}_n \equiv b_n(\gamma_0)$ and their derivatives. For brevity, we have suppressed the argument γ_0 in these functions.

n	b_n	$-\gamma_{N-1}$
2	$\bar{b}_2 + \gamma_1\bar{b}_1' + \frac{1}{2}\gamma_1^2\bar{b}_0''$	$\bar{b}_1'/\bar{b}_0''$
3	$\bar{b}_3 + \gamma_2\bar{b}_1' + \gamma_1\bar{b}_2' + \gamma_1\gamma_2\bar{b}_0'' + \frac{1}{2}\gamma_1^2\bar{b}_1'' + \frac{1}{6}\gamma_1^3\bar{b}_0^{(3)}$	$(\bar{b}_2' + \gamma_1\bar{b}_1'' + \frac{1}{2}\gamma_1^2\bar{b}_0^{(3)})/\bar{b}_0''$
4	$\bar{b}_4 + \gamma_3\bar{b}_1' + \gamma_2\bar{b}_2' + \gamma_1\bar{b}_3' + (\frac{1}{2}\gamma_2^2 + \gamma_1\gamma_3)\bar{b}_0''$	$(\bar{b}_3' + \gamma_2\bar{b}_1'' + \gamma_1\bar{b}_2'' + \gamma_1\gamma_2\bar{b}_0^{(3)}$
	$+\gamma_1\gamma_2\bar{b}_1'' + \frac{1}{2}\gamma_1^2\bar{b}_2'' + \frac{1}{2}\gamma_1^2\gamma_2\bar{b}_0^{(3)} + \frac{1}{6}\gamma_1^3\bar{b}_1^{(3)} + \frac{1}{24}\gamma_1^4\bar{b}_0^{(4)}$	$+\frac{1}{2}\gamma_1^2\bar{b}_1^{(3)} + \frac{1}{6}\gamma_1^3\bar{b}_0^{(4)})/\bar{b}_0''$

TABLE 25.2 Coefficients of the successive extension of the expansion coefficients in Eq. (25.182) for $n = 3$ determined from $M = 1, 2, 3, 4$ strong-coupling coefficients (4, 8, −16, 160) of Eq. (25.183).

n	a_6	a_7	a_8	a_9
1	−203.827			
2	−5.67653	17.6165		
3	−4.25622	9.04109	−15.7331	
4	−3.80331	6.87304	−10.0012	12.3552

TABLE 25.3 Coefficients of the successive extension of the expansion coefficients in Eq. (25.182) for $n = 4$ determined from $M = 1, 2, 3, 4$ strong-coupling coefficients (4, 0, 0, 221.096) of Eq. (25.183).

n	a_6	a_7	a_8	a_9
1	−147.508			
2	−7.91064	37.1745		
3	−4.59388	12.3044	−27.0837	
4	−3.72613	7.47851	−12.2129	16.9547

25.8 RELATION BETWEEN σ-MODEL AND QUANTUM MECHANICS OF POINT PARTICLE ON SPHERE

For D=1, the coordinate x may be identified as a time t and the field variable $\pi_a(t)$ as a normalized position variable $x^a(t)$ of a massive point particle on the surface of a sphere. Then the action (25.228) for $t = 2/R$ describes the quantum mechanics of this system. It has the general geometric form

$$\mathcal{A} = \frac{1}{2}\int dt\, g_{ab}\dot{x}^a(t)\dot{x}^b(t), \qquad a, b = 1, \dots, L-1. \tag{25.189}$$

TABLE 25.4 Coefficients of the successive extension of the expansion coefficients in Eq. (25.182) for $n = 5$ determined from $M = 1, 2, 3, 4$ strong-coupling coefficients $(8, -8/3, 16/3, 106.131)$ of Eq. (25.183).

n	a_6	a_7	a_8	a_9
1	−108.648			
2	−10.1408	60.7217		
3	−4.75598	15.1045	−38.9689	
4	−3.57909	7.84272	−14.1142	21.6045

TABLE 25.5 Coefficients of the successive extension of the expansion coefficients in Eq. (25.182) for $n = 1$ determined from $M = 1, 2, 3, 4$ strong-coupling coefficients $(4, -24, 48, 3825.54)$ of Eq. (25.183).

n	a_6	a_7	a_8	a_9
1	−413.921			
2	−5.25285	12.1104		
3	−442759	12450066	−196950675	
4	−5.7343	13.7134	−25.226	38.0976

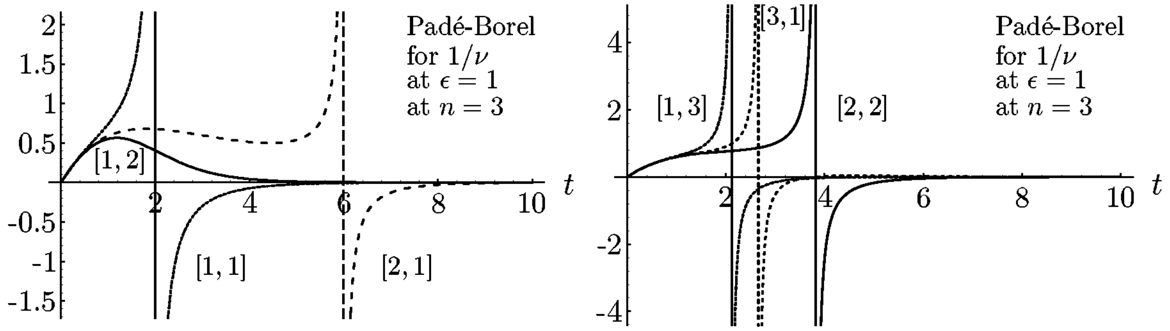

FIGURE 25.3 Integrands of the Padé-Borel transform (25.165) for the Padé approximants [1,1], [2,1], [1,2] and for [1,3], [3,1], [2,2] at $\epsilon = 1$ Only the last is integrable, yielding $\nu^{-1} \approx 1.25183 \approx 1/.79883$.

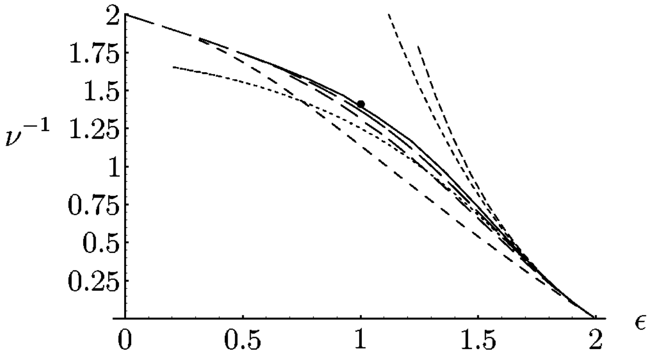

FIGURE 25.4 The inverse of the critical exponent ν for the classical Heisenberg model in the O(3)-universality class is plotted as a function of $\epsilon = 4 - D$ The solid curve is obtained from a variational interpolation of the five-loop ϵ-expansion of the ϕ^4-theory around $D = 4$ dimensions and the four-loop ϵ-expansion (25.162) of the nonlinear σ-model around 2 dimensions. The long-dashed curves are the successive approximations which make use of the strong-coupling expansion (25.183) only up to the first, second, and third order. The short-dashed curves display the first three and four terms of the ϵ-expansion and its Padé [1,2]-Borel approximations (the lowest curve). The dot corresponds to the seven-loop result in $D = 3$ dimensions, $\nu = 0.7096$ The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4)$ = (0.87917, 0.75899, 0.731431, 0.712152). These are extrapolated in Fig. 25.8 to infinite order, yielding $\nu = 0.705$.

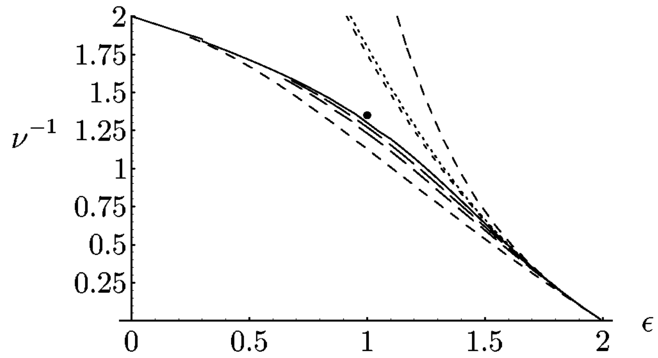

FIGURE 25.5 The inverse of the critical exponent ν for the O(3)-universality class is plotted as a function of $\epsilon = 4 - D$ The solid curve is obtained from a variational interpolation of the five-loop ϵ-expansion of the ϕ^4-theory around $D = 4$ dimensions and the four-loop ϵ-expansion (25.162) of the nonlinear σ-model around 2 dimensions. The long-dashed curves are the successive approximations which make use of the strong-coupling expansion (25.183) only up to the first, second, and third order. The short-dashed curves display the first three and four terms of the ϵ-expansion and its Padé [1,2]-Borel approximations (the lowest curve). The dot corresponds to the seven-loop result in $D = 3$ dimensions, $\nu = 0.7096$ The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.88635, 0.810441, 0.786099\, 0.768565)$. These are extrapolated in Fig. 25.9 to infinite order, yielding $\nu = 0.738$.

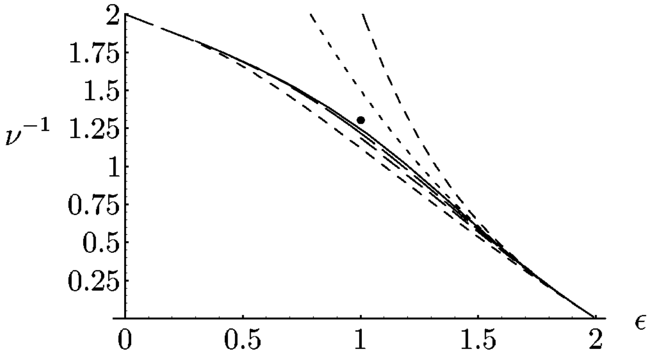

FIGURE 25.6 The inverse of the critical exponent ν for the O(5)-universality class is plotted as a function of $\epsilon = 4 - D$ The solid curve is obtained from a variational interpolation of the five-loop ϵ-expansion of the ϕ^4-theory around $D = 4$ dimensions and the four-loop ϵ-expansion (25.162) of the nonlinear σ-model around 2 dimensions. The long-dashed curves are the successive approximations which make use of the strong-coupling expansion (25.183) only up to the first, second, and third order. The short-dashed curves display the first three and four terms of the ϵ-expansion. There is no Padé-Borel approximation. The dot corresponds to the seven-loop result in $D = 3$ dimensions, $\nu = 0.767$ The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.89278, 0.842391, 0.820491, 0.802416)$. These are extrapolated in Fig. 25.10 to infinite order, yielding $\nu = 0.767$.

with a metric

$$g_{ab} = R^2\left(\delta_{ab} + \frac{x^a x^b}{1-\mathbf{x}^2}\right). \tag{25.190}$$

The Christoffel symbols defined via the inverse metric $g^{cd} = (g^{-1})^{cd}$ as

$$\Gamma_{ab}{}^{d} \equiv \frac{1}{2} g^{cd}\left(\partial_a g_{bc} + \partial_b g_{ac} - \partial_c g_{ab}\right) \tag{25.191}$$

has for (25.190) the simple form

$$\Gamma_{ab}{}^{d} = \frac{1}{R^2} g_{ab} x^d, \tag{25.192}$$

and the curvature tensor

$$R_{abc}{}^{d} \equiv \partial_a \Gamma_{bc}{}^{d} - \partial_b \Gamma_{ac}{}^{d} + \Gamma_{ac}{}^{f}\Gamma_{bf}{}^{d} - \Gamma_{bc}{}^{f}\Gamma_{af}{}^{d} \tag{25.193}$$

is found to be given by

$$\begin{aligned} R_{abcd} &= g_{de}R_{abc}{}^{e} = \frac{1}{R^2}\Big[(\delta_{bc}\delta_{ad} - \delta_{ac}\delta_{bd}) \\ &\qquad + \frac{1}{1-\mathbf{x}^2}\left(x^b x^c \delta_{ad} + \delta_{bc} x^a x^d - x^a x^c \delta_{bd} - \delta_{ac} x^b x^d\right)\Big]. \end{aligned} \tag{25.194}$$

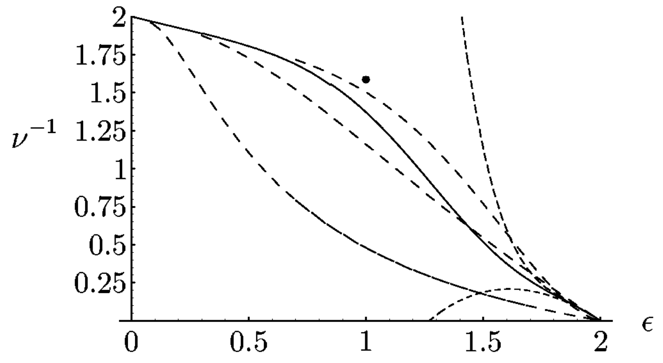

FIGURE 25.7 The inverse of the critical exponent ν for the O(1)-universality class (of the Ising model) is plotted as a function of $\epsilon = 4 - D$ The solid curve is obtained from a variational interpolation of the five-loop ϵ-expansion of the ϕ^4-theory around $D = 4$ dimensions and the four-loop ϵ-expansion (25.162) of the nonlinear σ-model around 2 dimensions. The long-dashed curves are the successive approximations which make use of the strong-coupling expansion (25.183) only up to the first, second, and third order. The short-dashed curves display the first three and four terms of the ϵ-expansion. There is no Padé-Borel approximation. The dot corresponds to the seven-loop result in $D = 3$ dimensions, $\nu = 0.6304$ The values from our successive interpolation are $(\nu_1, \nu_2, \nu_3, \nu_4) =$ (0.862357, 0.665451, 2.08686, 0.802416). Their position with respect to the accurate value $\nu = 0.767$ is shown in Fig. 25.11 showing the failure to converge up to order $M = 4$.

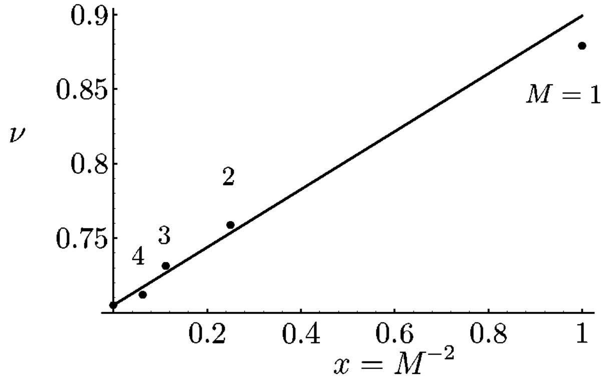

FIGURE 25.8 The three successive approximations $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.87917, 0.75899, 0.731431, 0.712152)$. for $n = 3$ (Heisenberg model) plotted as a function of $x = M^{-2}$ which makes them lie a straight line with the intercept $\nu_\infty = 0.705$.

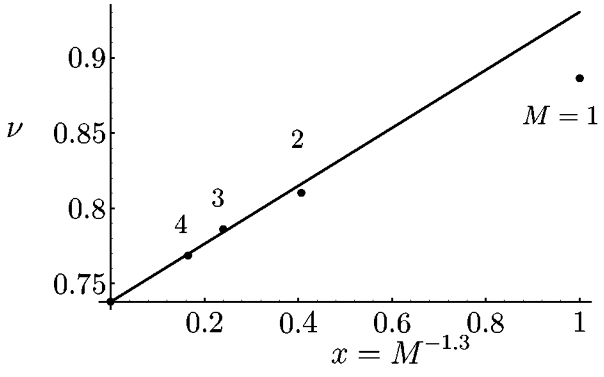

FIGURE 25.9 The three successive approximations $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.88635,\ 0.810441,\ 0.786099 0.768565)$ for $n = 4$ plotted as a function of $x = M^{-1.3}$ which puts them closest to a straight line with the intercept $\nu_\infty = 0.738$.

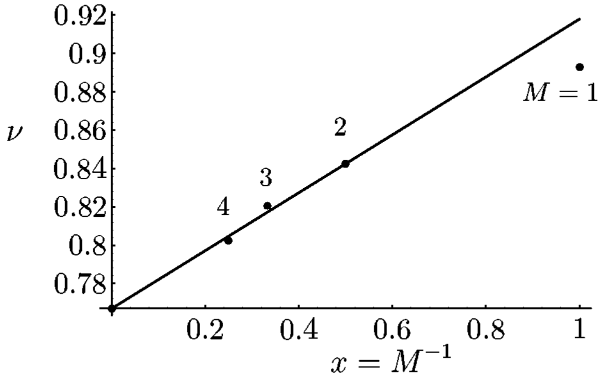

FIGURE 25.10 The three successive approximations $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.89278,\ 0.842391,\ 0.820491,\ 0.802416)$ for $n = 5$ plotted as a function of $x = M^{-1}$ which puts them closest to a straight line with the intercept $\nu_\infty = 0.767$.

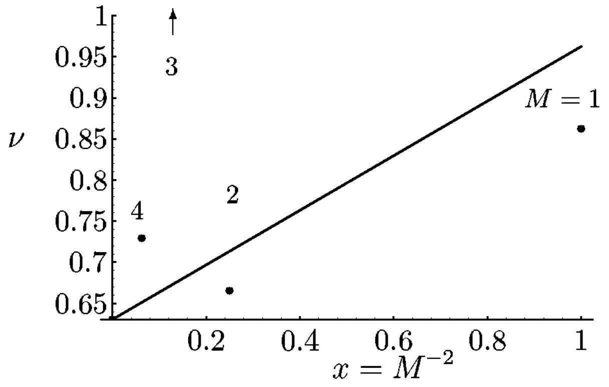

FIGURE 25.11 The three successive approximations $(\nu_1, \nu_2, \nu_3, \nu_4) = (0.862357, 0.665451, 2.08686, 0.802416)$. for $n = 1$ plotted as a function of $x = M^{-2}$ which puts them closest to a straight line with the intercept $\nu_\infty = 0.767$.

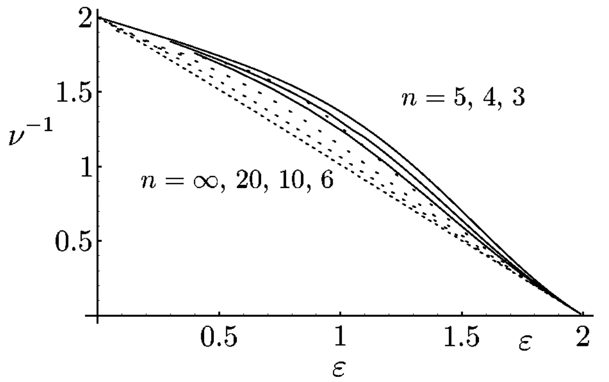

FIGURE 25.12 The highest approximations ($M = 4$) for $n = 3, 4, 5$ (counting from the top), and the $1/n$-expansions to order $1/n^2$ for $n = \infty, 20, 10, 6$ (counting from the bottom). The sixth-order result is obviously still far from the exact one.

Using (25.190), this can be expressed in the form typical for homogeous spaces:

$$R_{abcd} = \frac{1}{R^2}\left(g_{ad}g_{bc} - g_{ac}g_{bd}\right). \tag{25.195}$$

The Ricci tensor and curvature scalar are

$$R_{ab} = \delta^c{}_d R_{acb}{}^d = (N-2)g_{ab}, \qquad R = g^{ab}R_{ab} = \frac{(N-1)(N-2)}{R^2}. \tag{25.196}$$

The path integral associated with the action (25.228) can be solved exactly by time slicing.[15] The resulting time evolution amplitude has an energy spectrum given by the eigenvalues of the Hamilton operator

$$H = \frac{\hbar^2}{2MR^2}L^2, \tag{25.197}$$

where $\hbar^2 L^2$ is th square of the angular momentum operator in N dimensions under which the sphere is rotationally invariant. The eigenvalues of L^2 are $l(l+N-2)$ with $l = 0,\ 1,\ 2,\ \dots$. The spectrum of H coincides with that of curved-space Schrödinger operator

$$H = -\frac{\hbar^2}{2MR^2}\Delta, \tag{25.198}$$

where Δ is the Laplace-Beltrami operator

$$\Delta = \frac{1}{\sqrt{g}}\partial_\mu \sqrt{g} g^{\mu\nu}\partial_\nu \tag{25.199}$$

on surface of the sphere.

Let us investigate whether the above formal evaluation of the Feynman diagrams in the nonlinear σ-model produces the same energy spectrum. The answer will be negative: the spectrum emerging from the σ-model will turn out to be the spectrum of a particle *near* the surface of a sphere. That spectrum is obtained by time-slicing naively the continuous path integral

$$Z = \int \mathcal{D}n^a \mathcal{D}\lambda e^{-\frac{1}{2}\int d\tau\left\{\dot{n}_a^2 + \lambda\left[(n^a)^2 - 1\right]\right\}}, \tag{25.200}$$

in which a particle moves initially through an N-dimensional euclidean space, and is restricted to a sphere by the δ-functions. In the time-sliced version, the particle lies on the surface only at the points where the δ-function forces it to do so. The intermediate sections of paths, however, run straight through the N-dimensional space to the next point on the surface, thereby leaving the surface. This is why this path integral descibes aparticle *near* the surface of the sphere. The difference between the energies is explained in the reference in Footnote 15.

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[15] See Sections 8.9 and 10.4 in H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics*, World Scientific, Singapore, 1995.

The spectrum *near* the surface of a sphere in N dimensions is

$$E_l = \frac{\hbar^2}{2R^2}(L_2^2)_l, \tag{25.201}$$

with eigenvalues $(L_2^2)_l = (l+N/2-1)^2 - 1/4$ for $l = 0,\ 1,\ 2,\ \dots$ which have their origin in a large-argument expansion of a Bessel function

$$I_{l+N/2-1}(z/\epsilon) \approx \sqrt{\frac{2\pi z}{\epsilon}}e^{z/\epsilon}\left[1-\epsilon\frac{(L_2^2)_l}{2z}+\dots\right]. \tag{25.202}$$

These appears in the time slices of width ϵ of the exponential $e^{-\frac{1}{2}\int d\tau\left\{\dot{n}_a^2+\lambda\left[(n^a)^2-1\right]\right\}}$ when transforming the cartesian cordinates n_a the spherical coordinates in an N-dimensional space. On the sphere, the Hamiltonian operator (25.197) gives the energy spectrum

$$E_l = \frac{\hbar^2}{2R^2}(L^2)_l, \tag{25.203}$$

where $(L^2)_l = l(l+N-1)$ for $l = 0,\ 1,\ 2,\ \dots$. The difference between the energies near and on the sphere has the l-independent value

$$\Delta E_l = \frac{\hbar^2}{2R^2}\frac{(N-1)(N-3)}{4}. \tag{25.204}$$

The lowest-order calculation of the renormalization constants in the nonlinear σ-model shows that this calculation procedure produces a spectrum of the type (25.201).

To see this we consider the renormalized action (25.48) and observe that the squared mass of the π-field is modified by the factor Z_h of Eq. (25.51). For the mass m itsself, this implies

$$m_R = m\left(1+\frac{\hbar}{R^2}\frac{N-3}{4}L+\dots\right), \tag{25.205}$$

where we have replaced t by $1/R^2$ and reinserted $\hbar$, thus returning to proper physical units. The Feynman integral (25.38) for L can easily be performed for $D = 1$ using the formula $\int dp/(p^2+m^2) = \pi$, yielding $L = 1/2m$ [compare also (9.122)]. The mass receives therefore an explicit correction

$$m_R = m + \frac{\hbar}{2R^2}\frac{N-3}{4}+\dots\ . \tag{25.206}$$

The quantum mechanical ground state energy of a harmonic oscillator of frequancy m_R is $m_R\hbar/2$. The ground state energy of th $N-1$ harmonically fluctuating variables $x_a(\tau)$ is therefore

$$E = (N-1)\frac{m_R\hbar}{2} = (N-1)\frac{m\hbar}{2}+\frac{\hbar^2}{2R^2}\frac{(N-1)(N-3)}{8}+\dots\ . \tag{25.207}$$

In the limit $m \to 0$, we remain with the ground state energy (25.201) *near* the sphere.

25.9 GENERALIZATION OF MODEL

There exists a simple generalization of a point particle on a surface of a sphere: The *spinning top*. In fact, the ordinary spinning top in three dimensions is equivalent to a point particle on the surface of a sphere in four dimensions.[16] The action of a symmetric spinning top with moments of inertia I is

$$\mathcal{A} = \frac{1}{2I}\int dt(\omega_1^2 + \omega_2^2 + \omega_3^2), \tag{25.208}$$

where ω_i are the angular velocities of the spinning top. If $g = e^{-i\varphi(t)\sigma/2}$ denote the 2×2 -rotation matrices specifying the orientation of the top, they are defined by

$$\omega_i = i\mathrm{tr}\,(\sigma_i g^{-1}\partial_t g). \tag{25.209}$$

Alternatively we can write

$$\mathcal{A} = \int dt \frac{1}{I}\mathrm{tr}\,[(g^{-1}\partial_t g)^2], \tag{25.210}$$

This system has a field theoretic analog in a generalized nonlinear σ-model defined by the action

$$\mathcal{A} = \frac{1}{t}\int d^Dx\,\mathrm{tr}\,[g^{-1}\partial_\mu g\, g^{-1}\partial^\mu g]. \tag{25.211}$$

The partition function (25.14) including an external magnetic field of the type (25.20) becomes for this action

$$\begin{aligned} Z \;=\; & \int \mathcal{D}g \exp\Big\{-\frac{1}{t}\int d^Dx\,\mathrm{tr}\,[g^{-1}\partial_\mu g\, g^{-1}\partial^\mu g] + h\,\mathrm{tr}\,[D(g) + D^*(g)] \\ & \qquad -\frac{1}{2a^D}\int d^Dx \log\det g\Big\}, \end{aligned} \tag{25.212}$$

where $D(g)$ is some matrix representation of the group elements g. In general, we may assume g to be elements of any Lie group which can be represented as exponentials

$$g = e^{-i\pi_a G_a}, \tag{25.213}$$

where the generators G_a close under commutations relations, with antisymmetric structure constants f_{abc}:

$$[G_a, G_b] = if_{abc}G_c. \tag{25.214}$$

From the exponential form we find the partial derivatives $g^{-1}\partial_\mu g$ as

$$g^{-1}\partial_\mu g = e^{i\pi_a G_a}\frac{1}{d\pi_a}\left[e^{-i(\pi_a + d\pi_a)G_a} - e^{-i\pi_a G_a}\right]. \tag{25.215}$$

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[16] See Chapter 1 in the reference quoted in Footnote 15.

The exponential $e^{i\pi_a G_a} e^{-i(\pi_a+d\pi_a)G_a}$ is expanded in a the Neumann-Liouville or Dyson series [recall (1.143)]. Abbreviating $\pi_a G_a$ by $\not\pi$, this gives

$$\begin{aligned} e^{i\not\pi}\, e^{-i(\not\pi_a+d\not\pi)} &= 1-i\int_0^1 d\sigma\, e^{i\sigma\not\pi}\, d\not\pi\, e^{-i\sigma\not\pi} + \mathcal{O}(d\not\pi^2) \\ &= 1-i\left\{d\not\pi + \frac{i}{2!}[\not\pi, d\not\pi] + \frac{i}{3!}[\not\pi,[\not\pi,d\not\pi]]+\dots\right\}.. \end{aligned} \tag{25.216}$$

In this way we find

$$g^{-1}\partial_\mu g = -iG_a\left(\partial_\mu\pi_a + \frac{1}{2}\pi_b\partial_\mu\pi_c\, f_{abc} + \frac{1}{6}\pi_b\pi_c\partial_\mu\pi_d\, f_{bde}f_{efa}+\dots\right). \tag{25.217}$$

Normalizing the generators to

$$\mathrm{tr}\,(G_aG_b) = \frac{1}{2}\eta_{ab}, \qquad \eta_{ab}\equiv f_{acd}f_{bcd}, \tag{25.218}$$

we obtain

$$\mathrm{tr}\,[g^{-1}\partial_\mu g\, g^{-1}\partial^\mu g] = \frac{1}{2}g_{ab}(\pi)\partial_\mu\pi_a\partial^\mu\pi_b, \tag{25.219}$$

with the metric in field space

$$g_{ab}(\pi) = \delta_{ab} - \frac{1}{12}f_{acd}f_{bce}\pi_d\pi_e - \frac{1}{360}f_{acd}f_{cpe}f_{phf}f_{bhk}\pi_d\pi_e\pi_f\pi_k+\dots\,. \tag{25.220}$$

From this we calculate the connection

$$\Gamma_{abc} = -\frac{1}{12}f_{cad}f_{bde}\pi_e+\dots\,, \tag{25.221}$$

and the curvature tensor (25.193) as

$$R_{abcd} = \frac{1}{12}(f_{ach}f_{bdh} - f_{bch}f_{adh})+\dots\,. \tag{25.222}$$

The expansion (25.220) starts therefore out like

$$g_{ab} = \delta_{ab} - R_{adbe}\pi_d\pi_e+\dots\,. \tag{25.223}$$

The commutation relations (25.214) are satisfied by the adjoint representation

$$(G_a)_{bc} = -if_{abc}, \tag{25.224}$$

which allows us to rewrite (25.225) as

$$R_{abcd} = \frac{1}{12}f_{abe}f_{ecd}+\dots\,. \tag{25.225}$$

In the tensor form of the adjoint representation, the generatos are

$$(G_{ab})_{cd} = if_{abe}f_{ecd}, \tag{25.226}$$

so that we may identify $R_{abcd} = -i(G_{ab})_{cd}$. In the case of the Lorentz group, the generators (25.226) become $(G_{ab})_{cd} = i(g_{ac}g_{bd} - g_{bc}g_{ad})$ as in Eq. (3.61), and (25.225) coincides with (25.195).

The perturbation expansion and critical behavior of this theory can be discussed in complete analogy with the previous O(N)-sigma model. One separates the action (25.228) in the coordinates $\pi^a(t)$ into free and interacting parts as

$$\begin{aligned} \mathcal{A} &= \frac{1}{2}\int dt\, \delta_{ab}\dot{\pi}^a(t)\dot{\pi}^b(t), \qquad a,b = 1,\dots,N-1, & (25.227)\\ \mathcal{A}^{\rm int} &= \frac{1}{2}\int dt\, R_{adbe}\dot{\pi}^a(t)\dot{\pi}^b(t)\,\pi^d(t)\pi^e(t), & (25.228) \end{aligned}$$

and obtains the first-order correction to the free-particle energy density

$$E^{(1)} = \langle \mathcal{A}^{\rm int}\rangle = -\frac{1}{2}R_{adbe}\langle\dot{\pi}^a(t)\dot{\pi}^b(t)\rangle\langle\pi^d(t)\pi^e\rangle(t) \qquad (25.229)$$

With a small infrared regulator mass m, the correlation function is

$$\langle\pi^a(t)\,\pi^a(t')\rangle = \int_{-\infty}^{\infty}\frac{dq}{2\pi}e^{iqt}\frac{1}{q^2+m^2} = \frac{1}{2m}e^{-m|t-t'|}, \qquad (25.230)$$

and yields the expectation values

$$\langle\pi^d\,\pi^e\rangle = \delta^{de}\frac{1}{2m}, \qquad \langle\dot{\pi}^a(t)\dot{\pi}^b(t)\rangle = -\delta^{ab}\frac{m}{2}, \qquad (25.231)$$

the latter in dimensional regularization where $\int dk/2\pi = 0$ so that the Jacobian in the measure of path iintegration can be ignored. Inserting this into (25.232), we obtain

$$E^{(1)} = \langle\mathcal{A}^{\rm int}\rangle = \frac{1}{8}R. \qquad (25.232)$$

Notes and References

For a derivation of the critical exponents of the O(N) nonlinear σ-model see
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J.C. LeGuillou and J. Zinn-Justin, Phys. Lett. B **21**, 3976 (1980).

For the perturbative analysis of the critical behavior of the generalized σ-model defined in Section 25.9 see
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